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INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(51) International Patent Classification 6:

G06F 159:00

(11) International Publication Number:

WO 97/41526

(43) International Publication Date:

6 November 1997 (06.11.97)

(21) International Application Number:

PCT/US97/07218

A1

(22) International Filing Date:

28 April 1997 (28.04.97)

(30) Priority Data:

08/641,071

26 April 1996 (26.04.96)

US

(71) Applicant: THE SCRIPPS RESEARCH INSTITUTE [US/US]; 10666 North Torrey Pines Road, La Jolla, CA 92037 (US).

(72) Inventors: WILSON, Ian, A.; 1025 Newkirk Drive, La Jolla, CA 92037 (US). LIVNAH, Oded; 5240 Fiore Terrace #3114, San Diego, CA 92122 (US). STURA, Enrico, A.; 5172 Park West Avenue, San Diego, CA 92117 (US). JOHNSON, Dana, L.; 1343 Lonely CoHage Road, Upper Black Eddy, PA 18972 (US). JOLLIFFE, Linda, K.; 16 Davenport Way, Belle Mead, NJ 08502 (US).

(74) Agent: LAND, John; Fish & Richardson, P.C., 4225 Executive Square, Suite 1400, La Jolla, CA 92037 (US).

(81) Designated States: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, ARIPO patent (GH, KE, LS, MW, SD, SZ, UG), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG).

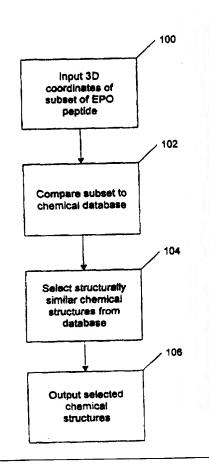
Published

With international search report.

(54) Title: SMALL MOLECULE MIMETICS OF ERYTHROPOIETIN

(57) Abstract

The invention features computer-assisted methods (100, 102, 104, 106, 200, 202, 204) for identifying molecules which will bind to the EPO receptor and act as an erythropoietin (EPO) mimetic. Preferred EPO mimetics identified using the method of the invention act as agonists of the EPO receptor in one or more in vitro or in vivo biological assays of EPO activity.



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SMALL MOLECULE MIMETICS OF ERYTHROPOIETIN

BACKGROUND OF THE INVENTION

1. Field of the Invention

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This invention relates to computer-assisted methods for identifying and designing small molecule mimetics of erythropoietin.

2. Description of Related Art

Erythropoietin (EPO) is the primary regulator of the proliferation and differentiation of immature erythroid cells. EPO is produced in the fetal liver and in the adult kidney in response to hypoxia (low oxygen levels in blood or tissue). It circulates in the blood stream where it targets the EPO receptor (EPOR) on committed progenitor cells in the bone marrow and other hematopoietic tissues. Recombinant human erythropoietin (rHuEPO) is widely used in therapy of patients with anaemia due to chronic renal failure, cancer chemotherapy and AZT treatment.

The EPO receptor belongs to the cytokine receptor superfamily which includes receptors for other hematopoietic growth factors such as interleukins (ILs), colony stimulating factors (CSFs) as well as growth hormone prolactin and ciliary neurotrophic factor (CNTF). The structural architecture of this family of receptors consists of three modules: a ligand binding extracellular domain, a short trans membrane region and a large cytoplasmic domain. It has been proposed that the extracellular domain of this superfamily comprises two discrete domains each containing approximately 100 residues that fold into a sandwich consisting of 7 antiparallel β-strands with the topology of an Ig constant domain. Members of the family share two characteristic motifs in their extracellular domain: a pair of conserved disulfide bridges in the N-terminal domain, and a WSXWS box (where X is any amino acid residue) in the C-terminal domain. For most members of this receptor superfamily, oligomerization of one or more polypeptide chains

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is essential for forming high affinity receptor complexes. A homodimer complex has been demonstrated to be the active form of hGHR and a similar model has been suggested for G-CSF, prolactin and EPO receptors.

Erythropoietin induces dimerization of two EPO receptor molecules, which results in subsequent phosphorylation of the cytoplasmic domains by the association with two tyrosine kinase (JAK2) molecules to initiate a cascade of events that leads to the relevant biological.

Given the importance of erythropoietin, it would be very desirable to be able to identify molecules capable of binding the EPO receptor and eliciting the response normally elicited by EPO.

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SUMMARY OF THE INVENTION

The invention features methods for identifying molecules which will bind to the EPO receptor and act as a EPO mimetic. Preferred EPO mimetics identified using the method of the invention act as agonists of the EPO receptor in one or more *in vitro* or *in vivo* biological assays of EPO activity. Preferred mimetics are molecules lacking peptide bonds, i.e., are non peptidic mimetics. Preferred peptide mimetics have 15 or fewer, more preferably 10 or fewer amino acids.

The methods of the invention entail identification and design of molecules having a particular structure. The methods rely on the use of precise structural information derived from x-ray crystallographic studies of the extracellular domain of EPO receptor (amino acids 1 to 225) complexed with a peptide, EMP1 (EPO Mimetic Peptide 1; described below), which acts as an EPO mimetic. This crystallographic data permits the identification of atoms in the peptide mimetic that are important for EPO receptor binding and dimerization. More importantly, this data defines a three dimensional array of the important contact atoms. Other molecules which include a portion in which the atoms have a similar three dimensional arrangement similar to some or all of these contact atoms are likely to be capable of acting as an EPO mimetic. Moreover, one can use the structural information to design or identify molecules having even more EPO activity than the peptide mimetic described herein.

The details of the preferred embodiment of the present invention are set forth in the accompanying drawings and the description below. Once the details of the invention are known, numerous additional innovations and changes will become obvious to one skilled in the art.

BRIEF DESCRIPTION OF THE DRAWINGS

FIGURE 1 is a flowchart showing a first method for identifying potential mimetics of erythropoietin using a computer system.

FIGURE 2 is a flowchart showing a second method for identifying potential mimetics of erythropoietin using a computer system.

Like reference numbers and designations in the various drawings indicate like elements.

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DETAILED DESCRIPTION OF THE INVENTION

Throughout this description, the preferred embodiment and examples shown should be considered as exemplars, rather than as limitations on the present invention.

Described below is the crystal structure of a small peptide mimetic of EPO bound to an peptide, EMP1 **EPO** receptor. The extracellular portion of the (GGTYSCHFGPLTWVCKPQGG; SEQ ID NO:1), is characterized by an intramolecular disulfide bridge. Several lines of evidence suggest that EMP1 can act as an EPO mimetic. For example, EMP1 competes with EPO in receptor binding assays and induces cellular proliferation of cell lines engineered to be responsive to EPO. Both EPO and peptide induce a similar cascade of phosphorylation events and cell cycle progression in EPO responsive cells. Furhter, EMP1 demonstrates significant erythropoietic effects in mice as monitored by two different in vivo assays of nascent red blood cell production. This data, when combined, strongly supports the notion that the peptide ligand, which has a sequence unrelated to that of EPO, is capable of binding to and inducing an agonist conformation or assembly of EPO receptor.

Design of small molecule mimetics

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The structure of the EMP1 dimer demonstrates that a molecule substantially smaller than the natural hormone can act as an agonist and induce the appropriate biological response. The peptide is assumed to have a substantially smaller contact interface with the receptor than its natural hormone. The binding determinants in the EPO receptor form an almost flat surface which is mainly hydrophobic in nature, without any cavities or charged residues that may help in design of a small molecule ligand to interact with the receptor.

This simplified framework of interactions revealed by the structural data presented herein can be used to identify additional EPO mimetics. The atoms of EMP1 which are important for binding to the EPO receptor and forming dimeric EPO receptor include those involved in the contact between the EMP1 (peptide) and EBP (EPO receptor) and

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those involved in contacts between the two EMP1 molecules in the dimeric complex (peptide-peptide contacts). In addition to the contacts listed in Table 2, the following EMP1-EMP1 hydrophobic contacts are significant: TyrP4, CysP6, PheP8, TrpP13, and CysP15 in each peptide. The following EMP1-EBP hydrophobic interactions are also significant: Tyr^{P4}, Phe^{P8}, and Trp^{P13} in each peptide. It will be understood by those skilled in the art that not all of the atoms present in a significant contact residue need be present in a mimetic. In fact, it is only those few atoms which actually from important contacts with the EPO receptor which are likely to be important for mimetic activity. Those skilled in the art will be able to identify these important atoms based on the model of the dimeric EMP1-EPO complex which can be constructed using the structural data herein.

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Preferred mimetics will include atoms at postions similar to those of the EPO receptor contacting atoms of EMP1. Even more preferred mimetics will be structurally similar to the dimer of EMP1 found in the structure described below. This is because the dimerization of EMP1 is an important factor in the diemerization of the EPO receptor.

The methods of the invention employ a computer-based methods for identifying 15 compounds having a desired structure. More specifically, the invention uses the threedimensional coordinates of subset of the atoms in the peptide GGTYSCHFGPLTWVCKPQGG when the peptide is co-crystallized with a portion of the erythropoietin receptor comprising amino acids 1 to 225 of the human EPO receptor, to determine peptide and non-peptide mimetic candidates by means of computer methods.

These computer-based methods fall into two broad classes: database methods and de novo design methods. In database methods the compound of interest is compared to all compounds present in a database of chemical structures and compounds whose structure is in some way similar to the compound of interest are identified. The structures in the database are based on either experimental data, generated by NMR or x-ray crystallography, or modeled three-dimensional structures based on two-dimensional (i.e., sequence)

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data. In de novo design methods, models of compounds whose structure is in some way similar to the compound of interest are generated by a computer program using information derived from known structures, e.g., data generated by x-ray crystallography and/or theoretical rules. Such design methods can build a compound having a desired structure in either an atom-by-atom manner or by assembling stored small molecular fragments.

The success of both database and *de novo* methods in identifying compounds with activities similar to the compound of interest depends on the identification of the functionally relevant portion of the compound of interest. For drugs, the functionally relevant portion is referred to a pharmacophore. A pharmacophore then is an arrangement of structural features and functional groups important for biological activity, *e.g.*, EPO activity.

Not all identified compounds having the desired pharmacophore will act as an EPO mimetic. The actual activity can be finally determined only by measuring the activity of the compound in relevant biological assays. However, the methods of the invention are extremely valuable because they can be used to greatly reduce the number of compounds which must be tested to identify an actual mimetic.

Dimerization of the EPO receptor is important for activity. Accordingly, preferred mimetics will be based on the structure of the EMP1 dimer as it is bound to the EPO receptor dimer. Thus, preferred mimetics have include important contacts from both of the RWJ 61233 peptides present in the structure described below. Such mimetics will favor dimerization of the EPO receptor.

Programs suitable for generating predicted three-dimensional structures from two-dimensional data include: Concord (Tripos Associated, St. Louis, MO), 3-D Builder (Chemical Design Ltd., Oxford, U.K.), Catalyst (Bio-CAD Corp., Mountain View, CA), and Daylight (Abbott Laboratories, Abbott Park, IL).

Programs suitable for searching three-dimensional databases to identify molecules bearing a desired pharmacophore include: MACCS-3D and ISIS/3D (Molecular Design Ltd., San Leandro, CA), ChemDBS-3D (Chemical Design Ltd., Oxford, U.K.), and Sybyl/3DB Unity (Tripos Associates, St. Louis, MO).

Programs suitable for pharmacophore selection and design include: DISCO (Abbott Laboratories, Abbott Park, IL), Catalyst (Bio-CAD Corp., Mountain View, CA), and ChemDBS-3D (Chemical Design Ltd., Oxford, U.K.).

Databases of chemical structures are available from Cambridge Crystallographic Data Centre (Cambridge, U.K.) and Chemical Abstracts Service (Columbus, OH).

De novo design programs include Ludi (Biosym Technologies Inc., San Diego, CA) and Aladdin (Daylight Chemical Information Systems, Irvine CA).

Those skilled in the art will recognize that the design of a mimetic may require slight structural alteration or adjustment of a chemical structure designed or identified using the methods of the invention.

- In general, chemical compounds identified or designed using the methods of the invention can be sythesized chemically and then tested for EPO activity using any of the methods described below. The methods of the invention are particularly useful because they can be used to greatly decrease the number potential mimetics which must be screened for EPO activity.
- The invention may be implemented in hardware or software, or a combination of both. However, preferably, the invention is implemented in computer programs executing on programmable computers each comprising a processor, a data storage system (including volatile and non-volatile memory and/or storage elements), at least one input device, and at least one output device. Program code is applied to input data to perform the functions

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described above and generate output information. The output information is applied to one or more output devices, in known fashion. The computer may be, for example, a personal computer, microcomputer, or workstation of conventional design.

Each program is preferably implemented in a high level procedural or object oriented programming language to communicate with a computer system. However, the programs can be implemented in assembly or machine language, if desired. In any case, the language may be a compiled or interpreted language.

Each such computer program is preferably stored on a storage media or device (e.g., ROM or magnetic diskette) readable by a general or special purpose programmable computer, for configuring and operating the computer when the storage media or device is read by the computer to perform the procedures described herein. The inventive system may also be considered to be implemented as a computer-readable storage medium, configured with a computer program, where the storage medium so configured causes a computer to operate in a specific and predefined manner to perform the functions described herein.

FIGURE 1 is a flowchart showing a first method for identifying potential mimetics of erythropoietin using a computer system. The method uses a programmed computer comprising a processor, a data storage system, at least one input device, and at least one output device, and comprises the steps of:

- (1) inputting into the programmed computer through an input device data comprising the three-dimensional coordinates of a subset of the atoms in the peptide GGTYSCHFGPLTWVCKPQGG when the peptide is co-crystallized with a portion of the erythropoietin receptor comprising amino acids 1 to 225 of the receptor, thereby generating a criteria data set (STEP 100);
- comparing, using the processor, the criteria data set to a computer database of chemical structures stored in the computer data storage system (STEP 102);

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- (3) selecting from the database, using a program suitable for searching threedimensional databases to identify molecules bearing a desired pharmacophore (such as those described above or equivalents), chemical structures having a portion that is structurally similar to the criteria data set (STEP 104);
- (4) outputting to an output device the selected chemical structures having a portion similar to the criteria data set (STEP 106).

FIGURE 2 is a flowchart showing a second method for identifying potential mimetics of erythropoietin using a computer system. The method uses a programmed computer comprising a processor, a data storage system, at least one input device, and at least one output device, and comprises the steps of:

- (1) inputting into the programmed computer through an input device data comprising the three-dimensional coordinates of a subset of the atoms in the peptide GGTYSCHFGPLTWVCKPQGG when the peptide is co-crystallized with a portion of the erythropoietin receptor comprising amino acids 1 to 225 of the receptor, thereby generating a criteria data set (STEP 200);
- (2) constructing, using a program suitable for generating chemical structure models (such as those described above or equivalents), a model of a chemical structure having a portion that is structurally similar to the criteria data set (STEP 202),
- (3) outputting to the output device the constructed model (STEP 204).

20 Confirmation of Biological Activity

In order to determine whether a molecule identified using the methods of the invention can act as an EPO mimetic, one or more *in vitro* or *in vivo* assays of EPO activity should be performed. For example, mimetic molecules should be able to stimulate proliferation of TF-1 cells (Kitamura et al., J. Cell Physiol. 140:323, 1985) or B6Sut cells (Greenberger et al., Proc. Natl. Acad. Sci. USA 80:2931, 1983), but preferably do not stimulate proliferation of cells which do not bear the EPO receptor. Thus, preferred mimetics do not stimulate proliferation of Mo7e cells (Avanzi et al., Br. J. Haematol. 69:359, 1988).

Potential mimetics can also be tested in a murine model of erythropoiesis. In this assay a potential mimetic is administered to normal mice which express endogenous basal levels of EPO. Reticulocytes are counted, preferably by flow cytometry, to determine whether the candidate mimetic increases reticulocyte levels. An increase in reticulocyte levels indicates that the candidate mimetic is stimulating erythropoiesis. Because the mice used in this assay already express EPO, this assay may be relatively insensitive. As an alternative, candidate mimetics can be assayed in the exhypoxic-polycythemic mouse bioassay. In this assay polycythemia is induced by conditioning mice in a hypobaric chamber to reduce endogenous EPO levels. A potential EPO mimetic can be administered to a conditioned mouse. Incorporation of ⁵⁹Fe into blood serves as a measure of erythropoiesis. This erythropoiesis can be attributed to the candidate mimetic.

The assays described above are examples of suitable assays. Other assays for EPO activity known to those skilled in the art are also useful.

In order to determine the biological activity of a candidate mimetic it is preferable to measure biological activity at several concentrations of candidate mimetic. The activity at a given concentration of candidate mimetic can be compared to the activity of EPO itself.

Structural Data

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The coordinates for amino acids 1 to 225 of the human EPO receptor bound to peptide EMP1 are presented in the attached appendix in standard Brookhaven database format. Also included in this appendix is a list of van der Waals interactions. These coordinates can be used in the design and identification of EPO mimetics according to the methods of the invention.

Structure of EBP-EMP1 Complex

The extracellular fragment of human EPO receptor (EPO binding protein, EBP), consisting of residues 1-225, was expressed in Escherichia coli and purified as described

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(Johnson et al., Protein Express. Purif. 7:104, 1996). Rhomboidal-shaped crystals of an EBP complex with EMP1 were obtained in orthorhombic space group P2,2,2, with cell parameters a=59.2Å, b=75.5Å, c=132.2Å, with two EBP and two peptide molecules in the asymmetric unit and a V_M=2.8 Å'/dalton (Matthews, J. Mol. Biol. 33:491, 1968). The crystal structure was determined by multiple isomorphous replacement (MIR) using two heavy atom derivatives (Table 1). Residues 1-2 and 19-20 of each peptide as well as residues 1-9, 21-23, 164-166, 221-225 of receptor molecule I, and residues 1-9, 21-23, 133-135, 221-225 of receptor molecule II had poor or no electron density and are excluded from the structure analyses

An important break in the electron density that affects the structure interpretation occurs for the three residues (Arg²¹ -Gly²² -Pro²³) that link the amino terminal α -helix to the first β-strand in D1 of both receptor molecules. A molecular packing diagram shows the proximity of a second non-crystallographically related dimer in the crystal that gives two possibilities of how this three-residue linker may be connected. The current choice of linker connectivity is based on a structure of another independent EBP-peptide complex at higher resolution (2.5 Å), which shares a similar molecular packing, but for which the electron density is clear for these three residues. At present there are no experimental data to verify whether this N-terminal \alpha-helix exists in solution or is a crystallization packing artifact. Notably, this helical region is not observed in the published structures of hGHbp (begins at residue 32; deVos et al., Science 255:306, 1992), PRLR (begins at residue 2, without any defined secondary structure until the first β-strand, residue 6; Somers et al., Nature 372:478, 1994), the INF-yRα (begins at residue 17; Walter et al., Nature 376:230, 1995) or the tissue factor (begins at residue 3 without any defined secondary structure until the first β-strand, residue 11; Muller et al., Nature 370:662, 1994).

The EBP monomer folds into two domains, D1 and D2, that form an L-shape with the long axis of each domain aligned at approximately 90° to each other; the overall molecular dimensions are 45 Å x 52 Å x 62 Å. The N-terminal domain (D1, residues 10-

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114) and C-terminal domain (D2, residues 119-220) are connected by a short four residue α-helix linker. Both domains are more closely related in overall topology to Fibronectin type-III (FBN-III) domains than to Ig domains (Bork et al., J. Mol. Biol., 242:309, 1994). The FBN-III fold is composed of two antiparallel β -pleated sheets, consisting of strands A, B, E and strands G, F, C and C', and is found in the two domains of the human growth hormone (de Vos et al., Science 255:306, 1992) and prolactin (Somers et al., Nature 372:478, 1994) receptors, the D1 and D2 domains of the α chain of interferon- γ receptor (IFN-γRα) (Walter et al., Nature 376:230, 1995), the D2 domain of CD4 (Wang et al, Nature 348:411, 1990; Ryu et al., Nature 348:419, 1990), the two domains of tissue factor (Muller et al., Biochemistry 33:10864, 1994; Harlos et al., Nature 370:662, 1994), the third fibronectin-type repeat of tenacin (Leagy et al., Science 258:987, 1992) and the D2 domain of the chaperone protein PapD (Holmgren et al., Nature 342:248, 1989). The FBN-III topology differs from an Ig constant domain by a shift of strand D from one β sheet (strands A, B, E and D) to the other (strands G, F, C, C'), where it is defined as the C' strand. Superposition of equivalent β -sheet core residues of the D1 and D2 domains in EBP gives an r.m.s. deviation of 2.3 Å for 77 Ca pairs, which is significantly larger than the corresponding domain overlaps for hGHbp (1.1Å) and PRLR (0.8Å), and reflects a difference in the subclass of fold between the two EBP domains.

In D1, a short α-helix (residues 10-20), precedes the first β-sandwich that is better described as a hybrid of the FBN-III fold with an Ig fold (residues 24-114), rather than strict FBN-III topology. In this h-type fold (Wang et al., Nature 348:411, 1990; Ryu et al., Nature 348:419, 1990), the C' strand is long and interacts first with strand C and then switches to interact with strand E (where C' changes its designation to strand D) forming a four-on-four strand β-sandwich. D1 contains the two conserved disulfide bridges linking Cys ²⁸ (βA) to Cys ³⁸ (βB) and Cys ⁶⁷ (βC') to Cys ⁸⁰ (βE). The number of residues between the cysteine pairs that form the two disulfide bridges are 9 and 15 for EBP, compared to 9 and 10 in both GHR and PRLR. The longer connection between strands C' and E enables the second half of strand C' to become strand D. This h-type topology is not found in either of the two s-type GHR domains. A potential glycoylation site exists

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on residue Asn^{52} which is located towards the end of the loop region connecting the βB and βC strands. Although Asn^{52} is not glycosylated in this bacterially expressed protein, an external cavity around the Asn^{52} side chain could easily accommodate a carbohydrate moiety.

A helical linker (residues 115-118) connects D1 to D2 (The φ, Ψ torsion angles for the interdomain helical linker for lle¹¹³, Asn¹¹⁴, Glu¹¹⁷ and Val¹⁸ are -50° -27°, -76°, -21°, -99°, 26°, and -151°, 38° respectively.) and has been observed in other members of this receptor family, hGHbp, PRLR, IFN-γRα and tissue factor. In EBP, the domain association is further restricted by a mixed assortment of hydrogen bonding, hydrophobic interactions and one salt bridge (between Arg²² and Asp¹²²) from 11 residues of D1 and 12 residues of D2 with a total buried surface [The molecular surface areas buried by interaction were calculated using the program MS (Connolly, J. Appl. Crystallog, 16:439, 1983) using a 1.7Å probe sphere and standard atomic radii (as described in Davies, et al, Ann. Rev. Biochem. 59:439, 1990). There may be some discrepancies between values reported here and other (deVos et al., Scince 255:306, 1992) published values due to use of a different algorithm (Connolly) vs. Lee et al., J. Mol. Biol., 55: 379, 1971) and probe radii. For clarity all values reported here have been calculated in the same way for better comparison between the receptors] of 950 Å² for the two domains.

D2 (residues 119-220) folds into the standard FBN-III (s-type) topology with one free cysteine and no disulfide bridges, consistent with GHR and PRLR that have three and two disulfide bridges, respectively, in D1 but none in D2. After the α -helix linker, D2 begins with an irregular coil (residues 118-126) that contains Pro^{124} which is conserved in the structures of hGHbp, PRLR, tissue factor and IFN γ -R α , and based on sequence alignment, in most class-1 and class-2 cytokine receptors (Bazan, Proc. Natl. Acad. Sci. USA 87:6934, 1990). This short coil ends with Gly¹²⁴ which has a positive ϕ (ϕ , $\Psi \approx 52^{\circ}$,40°) consistent with the equivalent Ala¹³⁶ and Ala¹⁰¹ torsion angles in hGHbp (ϕ , $\Psi \approx 63^{\circ}$,68°) and PRLR (ϕ , $\Psi \approx 58^{\circ}$,38°). The Pro¹²⁴ region forms an analogous extended bulge conformation adjacent and parallel to a corresponding bulge containing the

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WSXWS motif. The WSAWS sequence forms a modified wide β -bulge (Richardson, Adv. Prot. Chem. 34:167, 1981) and is located in an extended chain region immediately preceding the βG strand that would normally connect to the membrane spanning region of the EPOR.

The quaternary structure of the complex is composed of two peptides and two receptors that form a T-shapes assembly. A noncovalent peptide dimer interacts with two receptor molecules to generate an almost perfect 2-fold symmetrical arrangement. After superposition of D2 of the two EBP molecules in the dimer, the centers of mass of the two D1 domains are only 0.8 Å apart, sufficient to perturb perfect two-fold symmetry. Separate superposition of the corresponding D1 and D2 of each receptor in the dimer results in r.m.s. deviations of 0.53 Å (105 D1 Cα pairs) and 0.47 Å (93 D2 Cα pairs).

The cyclic EMP1 contains a single disulfide bridge between Cys^{P6} and Cys^{P15}, which links two short β-strands (residues 4-7 and 13-16) that are connected by a slightly distorted type 1 β -turn [Pro^{P10} (i+1) and Leu^{P11} (i+2) of the β -turn have ϕ , $\Psi \approx -62^{\circ}$, -38° and -99°, -60°, respectively. The carbonyl oxygen of LeuP11 has a hydrogen bond to EBP distorting the Ψ value from its normal 0°±30° (i+2) in a standard type I β -turn.] consisting of residues Gly^{P9}-Pro^{P10}-Leu^{P11}-Thr^{P12}. Each peptide has a very close association with its other peptide partner and buries 320 Å of its 1220 Å² molecular surface in this interaction (Connelly, J. Appl. Crystallog. 16:439, 1983; Davies et al., Ann. Rev. Biochem. 59:439, 1990; Richards, J. Mol. Biol. 55:379, 1971). Four hydrogen bonds between the mainchains of the two peptides results in formation of a four-stranded anti-parallel βpleated sheet (Table 2). Two symmetric hyrdophobic cores are assembled by peptide dimerization and are comprised of the disulfide bridges and the side chains of TyrP4, PheP8 and Trp^{P13}. The construction of each hydrophobic core resembles a box which places the aromatic rings of PheP8, TrpP13 and TyrP4 (from the other peptide) and the disulfide bridge (Cys^{P6}-Cys^{P15}) at the corners. The two glycine residues at either end of the peptide are not structured.

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The peptide dimer is embedded in a deep crevice between two EBP receptor molecules. A portion of each peptide monomer interacts with both receptor molecules. The binding sites of each EBP are practically identical due to the 2-fold symmetric interactions imposed on binding the peptide dimer. The four major contact areas on EBP come from segments on four loop regions (L1, L3, L5, L6) that connect strands A to B (L1 residues 33-34) and F to G (L6 residues 90-94) in D1 and strands B to C (L5 residues 148-153) and F to G (L6 residues 203-205) in D2. The total buried molecular surfaces in the peptide-EBP assembly are 840 Å² and 880 Å² for the two peptides and EBP's, respectively. The peptide-EBP interaction can be separated into distinct hydrophobic (67%) and polar (33%) areas. A hydrophobic core is formed between the peptide and receptor and comprises Phe93, Met150 and Phe205 from one EBP molecule and the peptide hydrophobic box consisting of PheP8 and TrpP13 from one peptide and TyrP4 and CysP15 from the other peptide. The polar interactions are located mainly at the bottom of the binding crevice and are mainly with loop L5 in D2. Five of the six hydrogen bonds are between the mainchain of the β-turn residues Gly^{P9}, Pro^{P10} and Leu^{P11} from one peptide with the mainchain and sidechain hydroxyl of conserved TyrP4, which crosses over its other peptide partner, to interact with loop L3 (Table 2). The EBP-EBP interaction makes a surprisingly minor contribution to the overall stability of the complex where the interreceptor buried molecular surface is only 75 Å², contributed by Leu¹⁷⁵ and Arg¹⁷⁸ from each receptor molecule.

EMP1 is one of a family of sequences that contain several conserved residues, besides the cysteines (**EXECUTED SECTION **EXECUTED SECTION **EXECU

Dimerization of EBP in Solution

To explore the interaction of EMP1 with EBP in solution we employed a [1,4-di-(2'-pyridyldithio DPDPB, reactive crosslinker bifunctionalsulphydryl propionamido) butane], in an attempt to stabilize a peptide-dependent dimeric structure. The choice of crosslinker was based on previous experiments with amine-reactive crosslinkers that were found to inactivate EBP. EBP contains a single free sulphydryl (Cys¹⁸¹) in D2 which is potentially reactive to crosslinking reagents (The DPDPB crosslinker itself does not inactivate the EPO binding potential of EBP nor the proliferative properties of EMP1). A dimeric EBP product is formed by co-incubation of EMP1, DPDPB and EBP. The amount of dimeric product increases with peptide concentration and no significant dimer product is observed in the absence of peptide. DPDPB-crosslinked products formed through disulfide-exchange reactions should be readily reversible by reduction as is seen for the covalently-linked EMP1-mediated dimer. Furthermore, we have constructed a covalently-linked dimeric form of EMP1 that demonstrates increased biological potency (Johnson et al, in preparation). The Cys¹⁸¹ residues in D2 of the EBP dimer are 20.7 Å apart (Sy-Sy distance) which approximates the 16 Å length (and approximately 2 Å in bond length at each end) of the DPDPB crosslinker. Thus EMP1 mediates formation of a soluble EBP dimer complex in solution consistent with the crystal structure.

The WSXWS motif

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The WSAWS sequence (residues 209-213) corresponding to the WSXWS box occurs in a β -bulge (Richardson, Adv. Prot. Chem. 34:167, 1981; Chan et al., Protein Science, 2:1574, 1993) immediately preceding β -strand G in D2. Residues in this motif do not interact with ligand, have no role in receptor-receptor interactions and are located on the opposite side of the receptor-receptor and receptor-ligand interface. The WSAWS box represents only a segment of a complex array of interactions that involves several other conserved side chains from the four-stranded β -sheet in D2. The indole ring systems of Trp²⁰⁹ and Trp²¹² point toward an external concave surface of the β -sheet and are only partially solvent exposed, whereas the Ala²¹¹ side chain points directly out into solution. The amides and hydroxyls of both Ser²¹⁰ and Ser²¹³ form hydrogen bonds with the main

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chain of residues 198 and 196 of adjacent strand F in a pseudo β -sheet type interaction that resembles a modified wide \beta-bulge (Richardson, Adv. Prot. Chem. 34:167, 1981; Chan et al., Protein Science, 2:1574, 1993) where the sidechain hydroxyl rather than the carbonyl oxygen makes the β -sheet interaction. The β -bulge architecture places the two Trp residues, which are spread four residues apart, on the same side of the β-sheet and not on opposite sides as in normal β -sheet or extended chain structures. The guanidinum group of Arg¹⁹⁷ from Strand F, the central residue (Richardson, Adv. Prot. Chem. 34: 167, 1981; Chan et al., Protein Science, 2:1574, 1993) in the bulge, is positioned exactly between the two Trp indole rings to form an extended π -cation system (Kumpf et al., Science 261:1708, 1993. The center of the pyrrole ring of Trp²⁰⁹, the NE of the Arg¹⁹⁷ and the center of the benzene ring of Trp212 are positioned on a straight line with the three planes of the conjugated systems stacked parallel to each other at approximately 4 Å spacing. In addition, the aliphatic portion of the Arg¹⁹⁹ side chain has hydrophobic interactions with the indole ring of Trp²⁰⁹, completing the alternating stacking of two aromatic and two positively-charged amino acid residues. The side chain of Glu¹⁵⁷ forms a hydrogen bond with Arg¹⁹⁷ presumably to help orient the guanidinium group and add some specificity and stabilization to the system.

It appears then that the linear WSXWS motif identified from sequence alignments of cytokine receptors represents only a component of a more complex conformational unit that contributes a significant structural feature to D2. Aromatic residues have previously been suggested to have a stabilizing effect and play a role as a folding nuclei in structures of antiparallel β -sandwiches (Finkelstein et al., Protein Eng. 6:367, 1993). The aminoaromatic parallel stacking between the guanidinium group of arginine and the aromatic rings is a common feature in protein structures (Burley et al., Adv. Prot. Chem., 39:125, 1988; Flocco et al., J. Mol. Biol., 235:709, 1994), but a parallel triple stacking of π -cation systems is rare (Kim et al., Biochemistry 32:8465, 1993) although observed in other class-1 cytokine receptors, hGHbp and PRLR.

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The structural equivalents of the WSXWS motif in hGHbp (YGEFS) and PRLR (WSAWS) are involved in an even more intricate and complex array of π -cation interactions. The π -cation system is extended in hGHbp and PRLR to include an additional aromatic residue (Trp186 for hGHbp and Trp156 for PRLR) from the loop region that links βC and $\beta C'$ in D2 and a positively-charged residue (Arg²¹¹ for hGHbp and Arg147 for PRLR) that stacks between the Trp and the second aromatic residue. The additional Arg residue is contributed either from the βF strand as in hGHbp (Arg²¹¹) or from BC as in PRLR (Arg147); the glutamine residue that hydrogen bonds and orients the arginine also switches strands. Sequence alignments suggest that this Arg-Gln switch could be common to other members of the class-1 cytokine receptor family. The extended π -cation system in hGHbp and PRLR consists of five positively charged and three aromatic residues stacked in an alternating order which comprises of Lys²¹⁵, Tyr²²², Arg²¹³, Phe²²⁵, Arg²¹¹, Trp¹⁸⁶, Lys¹⁷⁹ for hGHbp and Lys¹⁸⁵, Trp¹⁹¹, Arg¹⁸³, Trp¹⁹⁴, Arg¹⁴⁷, Trp¹⁵⁶, Lys¹⁴⁹ for PRLR. The first aromatic-Arg-aromatic trio are approximately 4Å apart, as in EBP, but the second system is stacked closer together at approximately 3.6 Å spacings consistent with π - π interaction (Burley et al., Adv. Prot. Chem., 39:125, 1988; Flocco et al., J. Mol. Biol., 235:709, 1994). The outer lysines also use the aliphatic portions of their side chains to form hydrophobic interactions with the aromatic rings. Based on sequence alignments with other members of the class-1 cytokine receptor superfamily, such structurally extended π -cation systems could exist in human thrombopietin, IL-6 and ciliary neurotrophic factor receptors, and in human IL-4 receptor based on structural modeling (Gustchina et al., Proteins 21:140, 1995). Although IFNγRα and tissue factor do not have a WSXWS motif, the corresponding sequences TTEKS (residues 213-217) for IFN-γRα (Walter et al., Nature 376:230, 1995) and KSTDS (residues 201-205) for tissue factor (Muller et al., Biochemistry 33:10864, 1994; Harlos et al., Nature 370:662, 1994), maintain a very similar β-bulge. The consensus sequence among these five x-ray structures indicates that a serine or threonine in positions 2 and 5 maintain a common set of hydrogen bonds between their side chain hydroxyls and the mainchain of the neighboring strand. Only in hGHbp is there no hydroxyl-containing residue in position 2, but Ser²²⁶ still maintains the equivalent interaction. A Ser²²⁶ to Ala

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mutation abrogates hGHR binding to hGH, and its expression on the cell surface is drastically reduced (Baumgartner et al., J. Biol. Chem., 269: 29094, 1994). In GM-CSFRα and IL-2Rβ, point mutations of the serine residues cause a substantial decrease in cell surface expression but little or no effect on ligand binding (Ronco et al., J. Biol. Chem. 269:277, 1994; Miyazaki et al., EMBO Journal 10:3191, 1991).

Conservation of the WSXWS motif in EPOR or its equivalent in other members of the class 1 cytokine receptors has been proposed to be essential for biological activity and was thus assumed to be part of the receptor binding site (Yoshimura et al., J. Biol. Chem. 267:11619, 1992; Quelle, Mol. Cell. Biol. 12:4553 1992). For EPOR, a systematic study of 100 mutations of the WSAWS sequence demonstrates that most of the mutations of the two tryptophan and serine resulted in molecules that did not reach the cell surface but were retained in the endoplasmatic reticulum (Hilton et al., Proc. Natl. Acad. Sci. USA 92:190, 1995; Hilton et al., J. Biol. Chem. 271:4699, 1996). Furthermore, an Ala²¹¹ to Glu mutation in the WSAWS sequence resulted in better transportation from the ER to the Golgi and a 3-5 fold increase of the number of EPOR molecules on the cell surface compared to the wild-type (Hilton et al., Proc. Natl. Acad. Sci. USA 92:190, 1995; Hilton et al., J. Biol. Chem. 271:4699, 1996). These results support our conclusion that the WSXWS sequence plays an important role in the structure and folding of D2 in EPOR and other related receptors.

Comparison with other cytokine-receptor complex structures

The overall quaternary structure of the peptide-EBP complex substantially from the equivalent arrangement in the hGH-hGHR complex. The non-symmetric nature of the single four-helix-bundle structure of the growth hormone ligand results in an asymmetric homo-dimerization of the receptor that corresponds to a 159° rotation between receptors compared to the almost perfect 2-fold (180°) rotation for the EBP-peptide complex. The tertiary arrangement of domains within EBP and hGHbp is also somewhat different. When the equivalent EBP and hGHbp D2 domains are superimposed on each other, their corresponding D1 domains differ by a 12° rotation and a 4.3Å translation.

The mechanism of hGH binding to its receptor has been well studied (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995) and is sequential. Initial high affinity (nM) binding of the hormone with one receptor results is a buried surface of 1130 Å² on the receptor. The second hGHbp2 has a substantially smaller interface (deVos et al., Science 255:306, 1992) with the second binding site on hGH and interacts only with the preformed 1:1 complex to generate buried surface areas of 740 Å² with hGH and 440 Å² with the first hGHbp1 (deVos et al., Science 255:306, 1992; (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995). The binding determinants of each hGHbp are comprised of the six recognition loops (L1-L6), three of which (L1-L3) come from one end of the β-sandwich structure in D1, one from the interdomain linker and two from D2.

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Although these two receptor complexes, EBP-EMP1 and hGH-hGHbp, have different dimeric arrangements, which probably in this case represent differences in the size and shape of the natural versus synthetic ligand, both receptors share equivalent ligand recognition loops, L1, L3, L5 and L6 for the EBP and L1 to L6 for the hGHbp. A nonactive PRLR, complexed with only one molecule of hGH, also uses the same contact loops (L1 to L6) (Somers et al., Nature 372:478, 1994). Based on similarity of the ligand recognition sites in hGHbp and PRLR, one would expect that the binding site of EBP, when its natural EPO ligand is bound, would extend to include two additional loops, L2 and L4, that comprise residues 59-63 (L2) between strands C to C', and residues 110-118 (L4) from the carboxyl end of βG in D1 and the interdomain linker. These six loops in EBP, hGHbp and PRLR area in structurally equivalent positions but vary in size, amino acid composition and conformation although the interacting portions of each loop (side or tip) remain similar; L1, L2, L3, L5 interact mainly with their tips and L6 with its side. In EBP, the L5 loop is three residues shorter than in hGHbp and PRLR, where the L6 loop is three and four residues longer than in hGHbp and PRLR, respectively. The L2 loop also varies (6 to 10 residues) among the three receptors but in EBP does not participate in peptide binding, and in hGHbp is partially disordered, although it does contact the hormone. In one respect, this situation is similar to the complementarity-

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determining regions (CDR's) in antibodies, where changes in length and sequence of the six binding loops impose specificity for different antigens, whereas the framework itself remains constant (Wilson et al., Ciba Foundation Symposium. Wiley, Chichester, 1991, Vol. 159, p. 13).

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It has been shown for the hGH-hGHbp complex that only a subset of 9 out of 33 interacting residues that make up the structural epitope of the receptor constitute a functional epitope or hot spot (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995) where high affinity binding interaction takes place. This reduced epitope is substantially smaller than the structural epitope and is comprised from residues (Arg⁴³, Glu⁴⁴, Ile¹⁰³, Trp¹⁰⁴, Ile¹⁰⁵, Pro¹⁰⁶, Asp¹⁶⁵, and Trp¹⁶⁹) which are located in contact loops L1, L3 and L5 with the most significant contribution (>4.5 kcal/mol) coming from two aromatic residues (Trp¹⁰⁴ and Trp¹⁶⁹) in L3 and L5 (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995; Wells, Proc. Natl Acad. Sci. USA 93:1, 1996). In EBP, Phe⁹³ is equivalent to Trp¹⁰⁴ in hGHbp, as suggested previously (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995; Wells. Proc. Natl Acad. Sci. USA 93:1, 1996; Jolliffe et al., Nephrol. Dial. Trans. 10:suppl. 2, 28, 1995), but there is no homologous residue to Trp¹⁶⁹ in the shorter L5 loop. In the EBP-EMP1 complex, the PheP8 peptide aromatic side chain occupies the equivalent position of the Trp169 side chain in hGHbp. One can assume that when EPO binds to its receptor, the hormone may provide an aromatic residue to the hydrophobic core of the binding interface and/or the L6 loop in EBP may play a more significant role in the hormone binding than in hGHbp, since it is 3 residues longer and contains the aromatic Phe²⁰⁵.

In these three class-1 receptor structures, some loops are disordered which are in D2 for EBP for EBP (residues 164-166 in EBP1 and 133-135 in EBP2) and in D1 for both hGHbp (residues 55-58, 73-78 for hGHbp1 and 54-60, 73-75 for hGHbp2) and PRLR (residues 31-33, 84-86). Otherwise, these three class-1 cytokine receptors do not differ greatly in their over all tertiary structures; D1 and D2 have broadly similar general

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arrangement in all three receptors such that the angle between the long axes of the two domains is approximately 90 degrees. I tis this arrangement of domains that allow these particular L1-L6 loops to be available for the recognition and binding of ligands. In a 2:2 complex between IFN-γ and its class-2 receptor IFN-γRα, D1 and D2 are related by a 125 degree angle, which elongates the receptor and restricts the binding determinants that can be used for interaction with hormone; the L1 loop now becomes buried in the D1-D2 interface, although the other five loops (L2-L6) are still available for ligand interaction. This elongated interdomain arrangement is also observed in tissue factor (Muller et al., Biochemistry 33:10864, 1994; Harlos et al., Nature 370:662, 1994) which has a distant relationship to the cytokine receptor superfamily.

A mutational analysis of the EBP molecule indicates that the most crucial amino acid residue for binding EPO is Phe⁹³ in the L3 loop (Jolliffe et al., Nephrol. Dial. Trans. 10:suppl 2,28, 1995). The Phe93Ala mutant shows an increase int he IC₅₀ compared to the wild-type by a factor of approximately 1000, whereas other mutants (Ser91Ala, Ser92Ala, Val94Ala, Met150Ala and His153Ala) show small relative increases in teh IC₅₀ of only 2.5-12.5 fold). The side chain of Phe⁹³ buries 66 Å² of molecular surface, which is the highest among interacting side chains. In hGHbp, the corresponding Trp104Ala mutation results in an increase in the K₄ by a factor of more than 2,500 compared to the wild-type indicating the equivalent importance of this residue in hGH binding and its key contribution to the hydrophobic core of the functional epitope (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995; Bass et al. Proc. Natl. Acad. Sci. USA 88:4498, 1991).

The role of dimerization on signal transduction

In the EBP-EMP1 complex structure, we surprisingly observe that a peptide, unrelated in sequence and probably in structure, to the natural ligand, can induce a biologically active dimerization of EPO receptor that promotes signal transduction and cell proliferation. Comparison of three class-1 cytokine receptor complexes, whose structures have been determined so far, suggests that when the natural EPO hormone, which is

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proposed to have a structure of a four-helix bundle (Boissel et al., J. Biol. Chem. 268:15983, 1993), induces receptor dimerization, it is more likely to resemble the hGH-hGHbp assemblage. This would suggest that more than one mode of productive extracellular dimerization is permissive for intracellular dimerization of the cytoplasmic domains with two JAK2 molecules in order to initialize the cascade of events that produces the biologically relevant signal (Ihle et al., Seminars in Immunology 5:375, 1993; Klingmuller et al., Cell 80:729, 1995). The peptide-EBP structure would then represent only one possible dimeric arrangement that promotes signal transduction.

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Mutant EPOR molecules, containing a single Arg to Cys mutation (Arg¹³⁰ in human and Arg¹²⁹ in murine), have been shown to form biologically active dimers in the absence of EPO (Yoshimura et al., J. Biol. Chem. 267:11619, 1992); Watowich et al., Proc. Natl. Acad. Sci. USA 89:2140, 1992; Watowich et al., Mol. Cell. Biol. 14:3535, 1994), suggesting that extracellular recptor homo-dimerization may be sufficient in itself for signal transduction. It has been shown in another system (Spencer et al., Science 262:1019, 1993) that activation of a specific set of transcription factors can be induced by the chemical crosslinking of cytoplasmic domains of modified cell membrane receptors that do not contain the extracellular and transmembrane domains. These receptors are not related to the cytokine receptor superfamily but illustrate that oligomerication plays a key role in activation of the receptor, and that the main functional role of the extracellular, ligand-binding domain is to allow (in the presence of ligand) dimerization or oligomerization and induce similar association of the cytoplasmic domains.

Mutageneses experiments originally suggested a role for the WSXWS motif in this cell signalling process (Yoshimura et al., J. Biol. Chem. 267:11619, 1992; Quelle et al. Mol. Cell. Biol. 12:4553, 1992; Chiba et al., Biochem. Biophys. Res. Comm. 184:485, 1992) possibly by promoting receptor homo-dimerization. However, truncation mutants of EPOR (Miura et al., Arch. Biochem. Biophys. 306:200, 1993) do not confirm this role for the WSXWS motif. The EBP-EMP1 complex structure shows that the WSXWS motif

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of the EPOR, as for the hGH-hGHbp complex (deVos et al., Science 255:306, 1992) is located on the opposite face of the molecule from the receptor dimerization. In the absence of unliganded structures for the extracellular domains of EPOR, hGHR and PRLR, it is not possible to determine whether any conformation change occurs on ligand binding that would involve the WSXWS box. Apart from being a striking structural feature in D2, and its obvious proximity to the membrane spanning domain, one cannot rule out possible interactions of this region with some other cell surface molecules that are involved somehow in the signal transduction process.

Towards design of small molecule mimetics

The structure of the EMP1 dimer demonstrates that a peptide considerably smaller than the natural hormone can act as an agonist and induce the appropriate biological response. The peptide can be assumed to form a substantially smaller contact interface than the natural hormone with the receptor. The peptide binding site in EBP forms an almost flat surface, which is mainly hydrophobic in nature, without any cavities or charged residues that are normally essential for the specific targeting of small molecule ligands to a receptor binding site. The hGHbp study (Wells et al., Science 267:383, 1995; Wells, Proc. Natl. Acad. Sci. USA 93:1, 1996) shows that only a small part of the observed structural binding site, the so-called functional epitope (supra), contributes most of the binding energy and strongly implied that a "minimized" hormone designed to interact with this site could form sufficient interactions to activate the receptor. Furthermore, the limited site of interaction of the small agonist peptide with the EBP corresponds almost exactly to the smaller functional epitope derived from alanine scanning of hGH and hGHbp. Thus, by a different approach, we have arrived at the similar conclusion that a small number of key interactions can contribute to a functional epitope on a receptor. Understanding of this simplified interaction surface can be now combined with further mutational studies to assist in identifying the most crucial residues in the functional epitope, and consequently provide a more practical target for drug design.

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The crystallographic data is summarized in Table 1. Native crystallographic data were collected on a Siemens multiwire area detector mounted on an Elliott GX-18 generator, operating at 40kV and 55mA, with a crystal-to-detector distance of 120mm. Two derivative data sets were collected on a MAR image plate mounted on a Siemens generator operating at 50kV and 80mA, with crystal-to-image plate distance of 150mm. Data were integrated, scaled and reduced using the programs XENGEN (Howard et al., J. App. Cryst. 20:383, 1987) for the native data and DENZO/SCALEPACK (Otwinowski et al., SERC Darsbury Laboratory, Warrington, 1993) for the derivative data. Initial multiple isomorphous replacement anomalous scattering (MIRAS) phases were calculated to 3.1 Å using the program package PHASES (Furey, American Crystallographic Association Fortieth Anniversary Meeting, New Orleans, LA, 1990) with a mean figure of merit of 0.64 (25.0-3.1 Å). Phases were refined in PHASES using the solvent flattening protocol to a mean figure of merit of 0.92 (25.0-3.1 Å). The quality of the map was generally good and most of the complex structure (94%) could be fitted using the graphics program O (Jone et al., Acta Crystallogr A47:110, 1991). The register of the amino acid residues was verified from the positions of the two disulfide bridges in D1. and the positions of the two Hg's from the mercury acetate derivative that were correctly assumed to bind to the free Cys¹⁸¹ residue. the peptide interpretation was verified from another data set from a complex between EBP and an iodinated peptide (TyrP4 was substituted for p-iodo-Phe), which diffracted to 3.3Å resolution, that in difference Fourier (Find-Fnut) and a clear indication of the location of the iodine atoms. The structure was refined using the slow-cooling protocol in X-PLOR 3.1(Brunger et al., Acta Crystallogr A46:585, 1990; Brunger, X-PLOR, Version 3.1: A System for X-ray and NMR, Yale Univ. Press, New Haven, CT, 1992) and rebuilt using Fo-Fc, 3Fo-2Fc and SIGMAA(Read, Acta Crystallogr. A42:140, 1986) weighted electron density maps. After every two cycles of refinement, a set of simulated annealing omit maps (7-10%) to reduce model bias was calculated and the entire structure rebuilt. After several cycles of refinement, individual temperature factors were calculated and after 10 cycles of refinement and model building, the R-value was 0.21 for 8.0-2.8 Å data with F>10 (13,984 reflections). The average thermal parameters for receptor I, receptor II and the

peptides are 10.5Å², 12.3Å and 10.7Å respectively. Only one non-glycine residue [Asn¹⁶⁴ in EBP2], located in a loop region in D1, is in a disallowed region in the Ramachandran plot. No solvent molecules were included in the model due to the moderate resolution (2.8 Å) of the structure determination.

5 Binding Contacts

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Binding contacts are summarized, in part, in Table 2: Hydrogen bond interactions in the binding site of the EBP-EMP1 complex. Due to the symmetrical nature of the complex, peptide-1 and peptide-2 have equivalent interactions with the two EBP molecules. The hydrogen bond interactions were analyzed using HBPLUS (McDonald et al., J. Mol. Biol. 238:777, 1994), based upon both distance (3.9 Å cutoff) and geometrical considerations.

A number of embodiments of the present invention have been described. Nevertheless, it will be understood that various modifications may be made without departing from the spirit and scope of the invention. Accordingly, it is to be understood that the invention is not to be limited by the specific illustrated embodiment, but only by the scope of the appended claims.

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EBP1	-PEPT	DE1							
VDW	1 LET		CB		PHE	308	CE1	1	3.95
VDW VDW	1 LEU 1 PHI		CB 、	4	PHE	308	CD1	1	4.11
VDW	1 PH		CE1	4	TRP TRP	313 313	CH2 CH2	1	3.74
VDW	1 PHI		.CZ	4	TRP	313	CZ2	1 1	3.98 4.08
VDW	1 PRO		CA	4	GLY		0	î	3.59
VDW VDW	1 PRO		CB	4	GLY		0	1	3.49
VDW	1 MET	_	C N	4	GLY PRO	309 310	0	1	3.66
VDW	1 MET		N	4	PRO	310	C	1 1	3.35 3. 6 2
VDW	1 MET		CA	4	LEU	311	0	ì	3.41
VDW VDW	1 MET		CA	4	GLY	309	0	1	3.78
VDW	1 MET		CA CG	4	LEU PHE	311	C CD2	1	3.87
VDW	1 MET		CG	4	PHE	308	CB CB	1 1	3.50 3.70
VDW	1 MET		CG	4	PHE	308	CG	1	3.79
VDW	1 MET		SD	4	PHE	308	CD2	ī	3.52
VDW VDW	1 MET		SD	4	THR	312	C	1	3.55
VDW	1 MET		SD SD	4	THR	312 313	CA	1	3.58
VDW	1 MET		SD	4	PHE	308	N CA	1 1	3.75 3. 9 1
VDW	1 MET	150	SD	4	PHE	308	CB	î	4.03
VDW	1 MET		CE	4	PHE	308	CD2	1	3.45
VDW VDW	1 MET		CE CE	4	TRP	313	CE2	1	3.71
VDW	1 MET		CE	4	PHE	308 313	CE2 CD2	1 1	3.79
VDW	1 MET		CE	4	TRP	313	NE1	1	3.83 3.91
VDW	1 MET		CE	4	TRP	313	CZ2	ī	4.10
VDW VDW	1 MET		C	4	LEU	311	0	1	3.41
VDW	1 THR	151	N CA	4	LEU PRO	311	0	1	3.45
VDW	1 THE		CB	4	PRO	310	0	1 1	3.82 3.56
VDW		151	OG1	4	LEU	311	CD2	1	3.43
VDW		151	OG1	4	LEU	311	CA	ī	3.91
VDW VDW	1 THR 1 SER		CG2	4	PRO	310	0	1	3.60
VDW	1 SER		CB ND1	4	LEU	311	0	1	3.54
SHORTVDW	1 HIS		CEl	4	THR	312	0 0G1	1	3.57 2. 8 7
VDW	1 HIS		CE1	4	THR	312	CB	ī	3.48
VDW	1 HIS		CE 1	4	THR		CA	1	3.76
VDW VDW	1 HIS		NE2 CE2	4	THR	312	OG1	1	3.57
VDW	1 PHE		CZ		PHE		CZ CE2	1	3.90
VDW	1 PHE		CZ	4	PHE	308	CZ	1	3.40 3.53
	BP2-PE		-	_					
VDW VDW		591 591	CA CB	4	TYR		OH	1	3.44
VDW		591	CB	4	TYR PRO		OH CB	1	3.88
VDW .	2 SER	591	OG	4	TYR		OH	1	3.95 3.44
VDW		591	OG	4	PRO	317	CB	ī	3.61
VDW		591	OG	4	TYR		CZ	1	3.83
VDW VDW		591 591	OG C	4	TYR		CE2	1	3.84
VDW		592	C N	4	TYR TYR		OH CE2	1	3.62
VDW	2 SER	592	N	4	TYR		CZ	1	3.66 3.68
VDW		592	CA	4	TYR	304	OH	ī	3.80
VDW VDW		592	CB	4	TYR		ОН	1	3.73
VDW		592 592	С О	4 4	TYR TYR		CE2	1	4.00
VDW		592	0	4	PRO		CE2 CD	1 1	3.53 3.59
VDW	2 PHE	593	CB	4	CYS		0	1	3.39
VDW	2 PHE		CD1	4	CYS	315	CB	1	3.55
VDW	2 PHE	593	CD1	4	TYR	304	CD2	1	3.72

	Thu Apr 25 15	:08:07 1996	2
all.con			1 3.90
	2 PHE 593 CD1 4 2 PHE 593 CE1 4	CYS 315 CB	1 3.71
12.1	2 FHE 555 CC1 4		1 3.17
SHORTVDW	2 VAL 594 CG1 4 2 VAL 594 CG1 4		1 3.23
SHORTVDW	-PEPTIDE2		
	1 SER 91 CB 4	PRO 417 CB	1 3.84
VDW VDW	1 SER 91 CB 4		1 3.90
VDW	1 SER 91 OG 4		1 3.90 1 3.82
VDW	1 SER 92 N 4		
VDW	1 SER 92 CA 4		1 3.85 1 3.42
VDW	1 SER 92 CB		1 4.04
VDW	1 251 25	1 TYR 404 CZ 1 TYR 404 CE2	1 4.09
VDW	1 351	4 CYS 415 0	1 3.43
VDW	1 1 1111	4 TYR 404 CE2	1 3.71
VDW	T END 33 COL	4 TYR 404 CD2	1 3.83
VDW	T FILL DO CO.	4 CYS 415 CB	1 3.92
VDW VDW	1 PHE 93 CE1	4 CYS 415 CB	1 4.08
VDW		4 TYR 404 CE2	1 4.09 1 3.54
VDW	1 VAL 94 CG1	4 PRO 417 CG	
VDW	1 VAL 94 CG1	4 PRO 417 CD 4 PRO 417 CG	1 3.54 1 4.11
VDW	1 VAL 94 CG2	4 PRO 417 CG	1
	-PEPTIDE2	4 PHE 408 CE1	1 3.14
SHORTVDW	2 LEU 533 CB 2 LEU 533 CB	4 PHE 408 CD1	1 3.77
VDW	2 LEU 533 CB 2 LEU 533 CB	4 PHE 408 CZ	1 4.00
VDW	2 LEU 533 CG	4 PHE 408 CE1	1 4.05
VDW VDW	2 LEU 533 CD1	4 PHE 408 CE1	1 3.75
VDW	2 LEU 533 CD1	4 PHE 408 CZ	1 3.92
VDW VDW	2 LEU 533 O	4 PHE 408 CE1	1 3.67 1 3.34
VDW	2 PHE 593 CE1	4 TRP 413 CH2	1 3.34 1 3.41
VDW	2 PHE 593 CE1	4 TRP 413 CZ2 4 TRP 413 CZ2	1 3.67
VDW	2 PHE 593 CZ	4 TRP 413 CZ2 4 TRP 413 CH2	1 3.96
VDW	2 PHE 593 CZ 2 PRO 649 CA	4 GLY 409 O	1 3.79
VDW	2 PRO 649 CA 2 PRO 649 CB	4 GLY 409 O	1 3.56
VDW VDW	2 PRO 649 C	4 PRO 410 O	1 3.72
VDW	2 MET 650 CA	4 PRO 410 O	1 3.59
VDW	2 MET 650 CA	4 GLY 409 O	1 3.67
VDW	2 MET 650 CA	4 LEU 411 0	1 3.77 1 3.80
VDW	2 MET 650 CG	4 PHE 408 CD2	1 3.92
VDW	2 MET 650 CG	4 PHE 408 CG 4 PHE 408 CB	1 4.05
VDW	2 MET 650 CG 2 MET 650 SD	4 PHE 408 CB 4 TRP 413 N	1 3.72
VDW	2 MET 650 SD 2 MET 650 SD	4 THR 412 C	1 3.75
VDW	2 MET 650 SD	4 PHE 408 CD2	1 3.76
VDW VDW	.2 MET 650 SD	4 THR 412 CA	1 3.78
VDW	2 MET 650 SD	4 PHE 408 CA	1 4.02
VDW	2 MET 650 CE	4 TRP 413 CE2	1 3.67 1 3.76
VDW	. 2 MET 650 CE	4 TRP 413 NE1 4 TRP 413 CD2	1 3.76
VDW	2 MET 650 CE	4 TRP 413 CD2 4 PHE 408 CD2	1 3.83
VDW	2 MET 650 CE 2 MET 650 CE	4 TRP 413 CD1	1 3.88
VDW		4 TRP 413 N	1 3.89
VDW VDW	2 MET 650 CE 2 MET 650 CE	4 TRP 413 CG	1 3.90
VDW VDW	2 MET 650 C	4 LEU 411 O	1 3.54
VDW	2 MET 650 C	4 PRO 410 O	1 3.57
VDW	2 THR 651 N	4 LEU 411 O	1 3.56
VDW	2 THR 651 N	4 PRO 410 C	1 3.77 1 3.41
VDW	2 THR 651 CA	4 PRO 410 0	1 3.41 1 3.03
SHORTV	OW 2 THR 651 CB	4 PRO 410 O 4 PRO 410 C	1 3.98
VDW	2 THR 651 CB 2 THR 651 CB	4 PRO 410 C 4 LEU 411 CA	1 4.02
VDW	2 THR 651 CB 2 THR 651 OG1	4 PRO 410 C	1 3.62
VDW	2 INC 001 001	* = 2.5 = = = = = = = = = = = = = = = = = = =	

all.con		7	Thu J	Apr 25	15	: 80 :	77 1	.996	3	
VDW	2	SER	652	N	4	LEU	411	ı c	1	3.83
VDW	2	SER	652	CA	4	LEU	411	LÖ	ī	3.51
VDW	2	SER	652	CB	4	LEU	411	L 0	1	3.18
VDW	2	SER	652	CB	4	LEU	411	L C	1	4.09
VDW	2	SER	652	OG-	4	THR	412		ī	3.73
SHORTVDW	2	HIS	653	.CE1	4	THR	412	2 OG1	1	3.00
VDW	2	HIS	653	CE1	4	THR	412	CB	1	3.91
PEP'	TII	DE1-F	PEPT:	IDE2						
SHORTVDW	3	THR	303	OG1	4	HIS	407	CB	1	2.94
VDW	3	THR	303	OG1	4	HIS	407	7 CA	1	3.61
VDW	3	TYR	304	CB	4	CYS	406	5 0	1	3.86
VDW	3	TYR	304	CD1	4	TRP	413	CZ3	1	3.81
VDW	3	TYR	304	CD1	4	TRP	413	CH2	1	3.94
VDW	3	TYR	304	0	4	CYS	406	5 N	1	3.33
VDW	3	TYR	304	0	4	CYS	406	5 0	1	3.47
VDW	3	TYR	304	0	4	SER	405	CA	1	3.57
VDW	3	SER	305	CA	4	TYR	404	1 0	1	3.51
VDW	3	SER	305	C	4	TYR	404	1 0	1	3.77
VDW	3	CYS	306	0	4	THR	403	3 CB	1	3.50
VDW	3	CYS	306	0	4	TYR	404	CB	1	3.54
VDW	3	CYS	306	0	4	TYR	404	CD1	1	3.59
VDW	3	CYS	306	0	4	TYR	404	A CA	1	3.75
VDW	3	CYS	306	CB	4	CYS	406	5 SG	1	3.81
VDW	3	CYS	306	SG	4	CYS	406	S SG	1	3.75
VDW	3	CYS	306	SG	4	CYS	406	5 CB	1	4.06
VDW	3	PHE	308	CEl	4	TYR	404	4 OH	1	3.93
VDW	3	PHE	308	CEl	4	TYR	404	4 CE1	1	4.08
VDW	3	TRP	313	CG	4	TRP	413	CD1	1	3.85
SHORTVDW	3	TRP	313	CD1	4	TRP	413	CD1	1	3.04
VDW	3	TRP	313	CD1	4	TRP	413		1	3.37
VDW	3	TRP	313	CD1	4	TRP	413	3 CG	1	4.09
VDW	3	TRP	313	NEl	4	TRP	41:		1	3.31
VDW	3	TRP	313	CZ2	4	CYS			1	3.84
VDW	3	TRP	313	CH2	4	CYS	41	5 SG	1	3.83
VDW	3	CYS	315	SG	4	TRP	413		1	3.59
VDW	3	CYS	315	SG	4	TRP	41	CE2	1	3.95
VDW	3	CYS	315	SG	4	TRP	41	3 CH2	1	4.00
VDW	3	GLN	318	CD	4	GLN	41		1	3.28
VDW	3	GLN	318	OE1	4	SER	40.	5 CB	1	3.80

bref2lc.pdb Thu Apr 25 12:27:47 1996

THE COMPLEX BETWEEN THE EXTRACELLULAR DOMAIN OF ERYTHROPOIETIS REMARK REMARK RECEPTOR (EBP) AND AN AGONIST EPO MIMETIC PEPTIDE 1 (EMF1) REMARK ***** WARNING **** RESIDUES 21-23 (521-522) and 164-166, 633-636 REMARK HAVE WEAK OP NO ELECTRON DENSITY MAP AND HAVE BEEN MODELED INTO THE STRUCTURE. THESE RESIDUES HAVE A HIGH B OF 90. REMARK REMARK THE STRUCTURE CONSISTS OF TWO RECEPTOR (RESIDUES 10-220, 510-720) REMARK AND PEPTIDE (RESIDUES 303-318, 403 418) MOLECULES.

1 N Lys 10 40.090 29.257 22.042 1. REMARK 1.00 22.57 10 1 MOTA 1.00 23.45 39.634 30.133 20.962 10 MOTA 2 CA LYS 38.753 29.361 19.979 1.00 22.87 : CB LYS 10 MOTA 3 18.735 1.00 22.92 38.334 30.155 MOTA 4 CG LYS 10 17.552 1.00 24.27 38,119 29.212 LYS CD 10 ATOM 17.890 1.00 26.55 28.015 10 37,165 6 CE LYS ATOM 17.998 1.00 26.18 35.685 28.367 LYS 10 NZ ATOM 31.427 21.420 1.00 22.91 38.921 10 LYS ATOM 8 С 39.589 32.442 21.636 1.00 24.17 9 0 LYS 10 MOTA 31.386 21.640 1.00 21.40 37.602 MOTA 10 N PHE 11 36.868 32.588 22.026 1.00 13.56 11 AO PHE 11 MOTA 32.257 22.725 1.00 19.07 35.549 12 CB PHE 11 ATOM 34.497 33.362 22.609 1.00 20.24 CG PHE 11 MOTA 13 34.862 34.717 22.670 1.00 19.49 CD1 PHE 11 MOTA 14 22.400 1.00 19.51 33.038 33.142 CD2 PHE 11 ATOM 35.728 22.527 1.00 19.64 33,910 CE1 PHE 11 ATOM 22.257 1.00 20.10 CE2 PHE 11 32.180 34.041 17 ATOM ..00 19.48 ..00 19.32 22.321 32.568 35.395 CZ. PHE 11 18 MOTA 33.567 22.887 PHÉ 11 37.644 С 19 ATOM 34.740 22.516 1.00 18.89 37.77€ PHE 11 0 ATOM 20 1.00 20.71 38.181 33.106 24.016 GLU 12 MOTA 21 N 38.905 34.036 24.886 1.00 20.59 12 CA GLU MOTA 22 39.253 33.423 26.246 1.00 21.48 GLU 12 ATOM 23 CB 40.185 34.309 27.123 1.00 23.60 12 GLU ATOM 24 CG 39.455 35.301 28.056 1.00 25.09 CD GLU 12 ATOM 25 40.024 36.417 28.275 1.00 23.07 OE1 GLU 12 ATOM 26 34.952 28.589 1.00 21.05 34.539 24.172 1.00 19.22 38.356 ATOM OE2 GLU 12 40.137 28 C GLU 12 ATOM 35.703 24.334 33.687 23.341 1.00 18.49 GLU 40.513 0 12 29 ATOM 40.730 1.00 17.67 13 N SER MOTA 30 41.903 34.094 22.571 1.00 16.71 CA SEP. 13 ATOM 31 42.522 32.898 21.851 1.00 18.51 ē 13 MOTA 32 CB SER 32.959 20.459 1.00 23.19 42.256 33 OG SEE 13 MOTA 41.570 35.202 21.554 1.00 15.57 34 С SER 13 MOTA 1.00 15.13 21.546 42.239 36.249 ATOM 35 0 SEF 13 40.563 34.355 20.698 1.00 12.00 36 N LYS 14 MOTA 40.117 35.912 19.675 1.00 8.51 37 CA LYS 14 MOTA 18.769 1.00 5.06 39.063 35.287 CB LYS 14 ATOM 38 34.366 17.714 39.629 1.00 2.36 ATOM 39 CG LYS 14 38.566 33.862 15.761 1.00 2.00 LYS MOTA 40 CD 14 ..00 15.496 2.27 39.191 33.270 LYS 14 41 CE. MOTA 32.742 14.528 1.00 2.00 NZ. LYS 14 38.193 42 ATOM 20.295 9.05 39.586 37.198 1.00 LYS 14 MOTA 43 C 39.782 38.290 19.755 1.00 7.15 LYS 14 ATOM 44 0 1.00 11.98 38.920 37.053 21.442 15 ATOM 45 N ALA 38.188 22.194 1.00 12.13 1.5 38.375 46 CA ALA ATOM 23.378 37.571 37.697 1.00 11.49 CB ALA 15 ATOM 47 39.592 38.960 22.666 1.00 12.49 48 ALA 15 MOTA 40.189 22.535 1.00 13.58 39.683 ALA 15 MOTA 49 38.207 23.167 1.00 13.97 40.560 MOTA 50 · N ALA 16 41.792 38.796 23.615 1.00 14.97 16 51 CA ALA MOTA 42.771 24.052 16 37.710 1.00 14.76 52 CB ALA ATOM 42.361 39.567 22.426 1.00 15.45 ALA 53 MOTA 40.759 42.624 22.537 1.00 15.35 O ALA 16 54 MOTA 1.00 16.12 42.444 38.896 21.274 LEU ATOM 5.5 N 17 43.007 39.467 20.042 1.00 15.92 ATOM 55 CA LEU 38.428 13.910 43.013 1.00 15.72 LEU 5.7 CB ATOM 18.662 44.204 37.485 1.50 17.46 MOTA 58 CG LEU 45.474 38.294 18.506 1.00 15.45 CD1 LEU ATOM 59 44.360 36.462 19.774 1.00 16.32 CD2 LEU MOTA 60 17 1.00 15.04 42.374 40.741 19.512 С LEU ATOM 61 41.438 18.711 1.00 15.91 42.985 ATOM 62 O LEU 19.908 41.136 41.013 1.00 17.34 ATOM 63 N LEU 18 19.443 CA LEU 18 40.434 42.210 .00 15.72 MOTA 38.999 41.367 19.022 1.00 13.72 ATOM 65 CB LEU 18 1.00 9.76 1.00 5.61 38.725 41.263 17.640 1.00 CG LEU MOTA 66 57 CD1 LEU 18 37.235 41.260 17.329 ATOM ..00 10.13 42.117 16.625 CD2 LEC 18 39.422 MOTA óà LEU 20.500 69 C 18 40.393 43.284 .00 17.38 MOTA ō. LEU 18 39.876 44.375 20.257 ATOM 70

bref21	c.pd	Ъ		Thu	Apr 25	12	:27:47	1996		2	
MOTA	71	N	ALA	19	40.9	21	42.981	21.680	1.00	19.88	7
ATOM	72	CA	ALA	19	40.9	25	43.941	22.789	1.00		ર્ક
MOTA	73	CB	ALA	19	41.5	60	43.331	24.041	1.00		6
ATOM	74	С	ALA	19	41.6		45.273	22.445	1.00	25.13	ઈ
ATOM	75	0	ALA	19	42.0		45.499	21.294	1.00	25.03	3
MOTA	76	N	ALA	20	41.6		46.164	23.453	1.00	28.77	7
ATOM	77	CA	ALA	20	42.2		47.514	23.333	1.00	28.51	ó
ATOM	7 B	CB	ALA	20	41.5		48.505	24.310	1.00	28.93	6
ATOM	79	C	ALA	20	43.7		47.526	23.562	1.00	27.54	6
ATOM	80	0	ALA	20	44.4		46.484	23.505		27.85	ŧ
ATOM	81	N	ARG	2:	44.3		48.699	23.848		90.00	7
ATOM	82	CA	ARG	21	45.7		48.784	24.075		90.00	5
ATOM ATOM	83 84	CB CG	ARG ARG	21 21	46.5 45.8		48.353	22.819		90.00	6
ATOM	85	CD	ARG	21	45.7		48.428 49.838	21.446		90.00	5
ATOM	86	NE	ARG	21	44.7		50.675	20.863 21.591		90.00 90.00	6 7
ATOM	87	cz	ARG	21	43.4		50.471	21.610		90.00	6
ATOM	88	NH1		21	42.9		49.448	20.926		90.00	7
ATOM	89	NH 2		21	42.6		51.270	22.350		90.00	7
ATOM	90	c	ARG	21	46.2		50.118	24.590		90.00	5
ATOM	91	0	ARG	21	45.8		51.199	24.132		90.00	8
ATOM	92	N	GLY	22	47.1		50.016	25.614		90.00	7
ATOM	93	CA	GLY	22	47.8	324	51.171	26.193		90.00	5
MOTA	94	С	GLY	22	49.0		51.371	25.314		90.00	ó
ATOM	95	0	GLY	22	48.9		51.174	24.089		90.00	3
ATOM	96	Ŋ	PRO	23	50.2	230	51.765	25.872		90.00	7
ATOM	97	CD	PRO	23	50.3	318	52.564	27.119		90.00	5
ATOM	98	CA	PRO	23	51.4	151	51.971	25.062	1.00	90.00	5
MOTA	99	CB	PRO	23	51.7	713	53.452	25.287	1.00	90.00	5
ATOM	100	CG	PRO	23	51.5		53.517	26.850	1.00	90.00	5
ATOM	101	С	PRO	23	52.6		51.167	25.544	1.00	90.00	٤.
ATOM	102	0	PRO	23	52.5		50.067	26.123		90.00	3
ATOM	103	N	GLU	24	53.6		51.758	25.308		28.27	7
ATOM	104	CA	GLU	24	55.1		51.178	25.741		24.32	ő
ATOM	105	CB	GLU	24	56.3		52.009	25.238		24.01	6
ATOM	106	CG	GLU	24	56.4		52.149	23.723		25.03	6
ATOM	107	CD	GLU	24	56.		50.822	22.959		24.22	6
ATOM	108	OE1		24	57.1		50.954	21.793		23.14	S
MOTA	109		GLU	24	56.4		49.692	23.478		18.50	5
ATOM	110	С	GLU	24	55.3		51.264	27.268		23.39	5
ATOM ATOM	111 112	0	GLU GLU	24 25	54.8 55.3		52.365	27.829		24.36	3
ATOM	113	CA	GLU	25			50.124	27.925		18.35	7
ATOM	114	CB	GLU	25	55.3 53.9		50.058 49.818	29.377		14.09	5
ATOM	115	CG	GLU	25	53.		49.985	29.907 31.410		17.09 22.21	5
ATOM	116	CD	GLU	25	53.		51.348	31.799		27.17	é
ATOM	117	OE1		25	53.		52.355	31.057		27.15	å
ATOM	118	OE2		25	52.		51.401	32.837		26.11	3
ATOM	119	c	GLU	25	56.		48.872	29.725		11.99	5
ATOM	120	ō	GLU	25	56.		47.779	29.181		14.38	8
ATOM	121	N	LEU	26	57.		49.098	30.572	1.00	8.48	-
ATOM	122	CA	LEU	26	58.		48.034	21.001	1.00	5.93	ž
ATOM	123	CB	LEU	26	59.	398	48.624	31.652	1.00	4.03	6
ATOM	124	CG	LEU	26	60.		47.880	31.488	1.00	2.00	÷
ATOM	125		LEU	26	61.		48.145	32.704	1.00	4.41	é
ATOM	126		LEU	26	60.		46.401	31.317	1.00	2.00	÷
ATOM	127	С	LEU	26	57.		47.188	32.030	1.00	6.68	-5
ATOM	128	.0	LEU	26	56.		47.727	33.041	1.00	9.43	3
atom	129	N	LEU	27	57.		45.880	21.797	1.00	5.17	7
ATOM	130	CA	LEU	27	56.		44.996	32.719	1.00	5.71	÷
ATOM	1,31	CB	LEU	27	55.		44.334	32.035	1.00	6.50	ć
MOTA	132	CG	LEU	2	54.		45.263	31.673		10.34	6
atom	133		LEU	2	53.		44.423	31.125		10.81	:
MOTA	134		LEU	27	53.		46.130	32.906	1.00	7.08	÷
ATOM	135	0	LET	27		454	43.923	33.397	1.00	7.41	1
ATOM	136	0	LEU	27		003	43.037	32.742	1.00	7.62	3
ATOM ATOM	137	N	CYS	28		460	43.964	34.726	1.00	7.42	:
ATOM	138	CA	CYS	28		208	43.027	35.554	1.00	4.67	5
atom atom	139	0	CYS	28		246	42.359	36.529	1.00	4.38	÷
ATOM	140 141	CB	CAS	28 28		217 26€	42.945	35.861	1.00	2.56	3
ATOM	142	SG	CYS	28		429	43.791 44.763	36.357 35.358	1.00	3.64	3.4
ATOM	143	14	PHE	23		599	41.153	35.336	1.00	4.37 2.00	16
ATOM	144	CA	PUE	29		817	40.403	37.943	1.00	2.00	.5
ATOM	145	CB	PHE	29		474	39.899	37.322	1.00	4.36	*7
ATOM	146	CG	PHE	29		58€	38.643	35.437	. 00	3.43	5
MOTA	147		PHE	29		493	37.369	36.990	1.00		
ATOM	148	CD2	2 PHE	29	55.	790	38.747	25.058	1.00		.;

bref21	c.pdb	Thu Ap	r 25 12	:27:47	1996	3
	149 CE1 PHE	29	55.605	36.243	36.206	1.00 2.00 6
MOTA		29		37.616	34.266	1.00 2.00 5
ATOM	-	29		36.365		1.00 2.00 6
MOTA	151 CZ PHE	29		39.260	38.543	1.00 3.80 €
MOTA	152 C PHE	29	_	38.897	37.957	1.00 2.00 ŝ
ATOM	153 O PHE			38.814	39.766	1.00 4.17 7
MOTA	154 N THR	30		37.694	40.463	1.00 3.12 5
MOTA	155 CA THR	30		38.116	41.820	1.00 2.00 6
ATOM	156 CB THE	30.	58.720		42.408	1.00 2.00 3
MOTA	157 OG1 THR	30	59.337	36.982		1.00 2.00 5
ATOM	158 CG2 THP.	30	57.763	36.661	42.827	1.00 6.81 6
ATOM	159 C THR	30	56.951	36.601	40.674	
ATOM	160 0 THR	30	55.774	36.924	40.814	
ATOM	161 N GLU	31	57.342	35.326	40.665	• • • • • • • • • • • • • • • • • • • •
ATOM	162 CA GLU	31	56.378	34.219	40.786	1.00 8.18 5
ATOM	163 CB GLU	31	56.577	33.240	39.650	1.00 7.89 6
ATOM	164 CG GLU	31	56.490	33.821	38.286	1.00 8.99 6
ATOM	165 CD GLU	31	56.651	32.750	37.248	1.00 10.58 6
ATOM	166 OE1 GLU	31	57.538	32.875	36.395	1.00 13.03 3
	167 OE2 GLU	31	55.916	31.753	37.302	1.00 14.01 3
ATOM	168 C GLU	31	56.453	33.432	42.079	1.00 8.38 6
ATOM		31	55.437	32.940	42.582	1.00 9.78 €
MOTA		32	57.678	33.064	42.416	1.00 7.19 7
MOTA			58.006	32.390	43.670	1.00 8.64 5
ATOM	171 CA ARG	32	58.844	31.154	43.405	1.00 9.16 5
ATOM	172 CB ARG	32		30.364	42.261	1.00 10.75 6
MOTA	173 CG ARG	32	58.284		42.469	1.00 11.21
ATOM	174 CD ARG	32	58.376	28.894		1.00 13.52 7
ATOM	175 NE ARG	32	57.070	28.271	42.295	
ATOM	176 CZ ARG	32	56.328	28.350	41.187	
ATOM	177 NH1 ARG	32	56.763	29.036	40.128	
ATOM	178 NH2 ARG	32	55.145	27.734	41.128	
ATOM	179 C ARG	32	58.834	33.536	44.224	1.00 9.21 6
ATOM	180 0 ARG	32	59.004	34.526		1.00 13.37 8
ATOM	181 N LEU	33	59.382	33.499		1.00 7.72 7
ATOM	182 CA LEU	33	60.084	34.736	45.716	1.00 8.01 6
ATOM	183 CB LEU	33	59.536	35.403	46 .98 6	1.00 7.85 6
ATOM	184 CG LEU	33	58.323	36.310	46.699	1.00- 2.00 6
	185 CD1 LEU	33	57.061	35.584	47.032	1.00 3.91 6
ATOM	186 CD2 LEU	33	58.381	37.604	47.464	1.00 2.00 6
ATOM		33	61.610	34.893		1.00 8.52 €
ATOM		33	62.269	35.702		1.00 10.67 8
ATOM		34	62.130	34.174		
MOTA	189 N GLU	34	63.539	34.21		
MOTA	190 CA GLU		64.315	33.00		
ATOM	191 CB GLU	34	63.518			_
ATOM	192 CG GLU	34				
ATOM	193 CD GLU	34	62.754			
ATOM	194 OE1 GLU	34	61.810			
ATOM	195 OE2 GLU		63.082			
MOTA	196 C GLU		63.678			
ATOM	197 & GLU		64.413			_
MOTA	198 N · ASP	35	62.978			
ATOM	199 CA ASP	35	62.981			
MOTA	200 CB ASP	35	62.215	34.03		
ATOM	201 CG ASP	35	60.678			
ATOM	202 OD1 ASP		60.05			
ATOM	203 OD2 ASE		60.102	2 33.91		5 i.00 2.00 E
ATOM	204 C ASE		62.33			6 1.00 3.42 5
MOTA	205 0 ASE		61.56	37.15		
ATOM	206 'N LE		62.67		16 23.83	4 1.00 2.00 7
ATOM	207 CA LET		62.09			7 1.00 2.00 5
MOTA	208 CB LEG		62.90			5 1.00 2.00 5
	209 CG LE		62.21			0 1.00 2.40 6
ATOM			60.99			
ATOM			63.18			
MOTA	211 CD2 LE		62.11			
MOTA	212 0 LE		63.07			
ATOM						
ATOM			61.03			
MOTA			60.96			
MOTA			59.86			
ATOM			60.00			
ATOM			59.95			
ATOM	219 C VA		60.55			
ATOM		L 37	59.73			
ATOM		s 38	61.20			
ATOM			60.B3	31 41.9		
ATOM			60.70			34 1.00 5.14 6
ATON			61.5			
ATOL			61.8			13 1.00 2.98 6
ATO			61.8		383 34.9	72 1.00 3.22 16

bref2	lc.p	dlb		Thu	Apr 25 1	4			
ATOM	227	N	PHE	39	59.811	42.540	30 740		_
ATOM	228	CA	PHE	39	59.621	42.507	30.742		7
ATOM	229	CB	PHE	39	58.865		29.286		5
ATOM	230	CG	PHE	39	57.461	41.225	28.900		Ę,
ATOM	231		PHE	39	56.416	41.198	29.411		5
ATOM	232		PHE	39	57.190	41.686	28.636		Ŧ
ATOM	233		PHE	39		40.807	20.709		٤.
ATOM	234		PHE	39	55.123	41.795	29.153		ŧ
ATOM	235	CZ			55.896	40.917	31.228	1.00 9.33	ξ.
			PHE	39	54.868	41.411	30.451	1.00 8.72	÷
ATOM	236	C	PHE	39	58.826	43.713	23.794		ŝ
ATOM	237	0	PHE	39	58.262	44.451	29.58 0		;
ATOM	238	И	TRP	40	58.837	43.926	27.490	1.00 3.45	7
MOTA	239	CA	TRP	40	58.084	44.996	26.846	1.00 4.71	Ē
ATOM	240	CB	TRP	40	58.826	46.352	26.872		=
ATOM	241	CG	TRP	40	60.014	46.517	25.928		
ATOM	242		TRP	40	61.386	46.185	26.200		ó
ATOM	243		TRP	40	62.143	46.555	25.062		5,
ATOM	244		TRP	40	62.049	45.595	27.294		5
ATOM	245		TRF	40	60.003	47.056	24.661	1.00 8.12	5
ATOM	246		TPP	40	61.277	47.087	24.144	1.00 6.99	
MOTA	247		TRP	40	63.527	46.358	24.98 9		ξ
ATOM	24B		TRP	40	63.431	45.395	27.217	1.00 10.61	
ATOM	249		TRP	40	64.152	45.780	26.068	1.00 11.43	
ATOM	250	С	TRP	40	57. 7 85	44.538	25.418	1.00 5.55	
ATOM	251	0	TRP	40	58.530	43.761	24.824	1.00 4.51	:
ATOM	252	Ŋ	GLU	41	56.625	44.914	24.914	1.00 7.38	•
ATOM	253	CA	GLU	41	56.267	44.533	23.556	1.00 8.54 8	5
ATOM	254	CB	GLU	41	54.898	43.940	23.555	1.00 7.91	
ATOM	255	CG	GLU	41	54.860	42.5B6	24.450	1.00 11.77	
ATOM	256	CD	GLU	41	53.619	41.687	24.254	1.00 13.67	
MOTA	257		GLU	41	53.418	40.748	25.055	1.00 15.11	
MOTA	258		GLU	41	52.843	41.891	23.301	1.00 17.90	
ATOM	259	С	GLU	41	56.335	45.715	22.558	1.00 9.08 6	
ATOM	260	0	GLU	41	56.456	46.888	22.956	1.00 8.71 3	
ATOM	261	N	GLU	42	56.403	45.389	21.271	1.00 8.40 7	
ATOM	262	A)	GLU	42	56.426	46.399	20.211	1.00 9.84	
ATOM	263	CB	GLU	42	57.729	47.207	20.227	1.00 6.56	
ATOM	264	CG	GLU	42	58.974	46.393	20.511	1.00 5.93	
ATOM	265	CD	GLU	42	60.242	47.114	20.115	1.00 7.01	
ATOM	266		GTf.	42	61.019	46.519	19.371	1.00 9.43	
ATOM	267	OE2	GLU	42	60.470	48.271	20.519	1.00 6.18 8	
ATOM	268	С	GLU	42	56.167	45.73?	18.853	1.00 9.90	
ATOM	269	0	GLU	42	5 5.88 0	44.532	18.795	1.00 9.59	
MOTA	270	N	ALA	43	56.243	46.514	17.771	1.00 10.98 7	,
ATOM	271	CA	ALA	43	55.988	46.007	16.400	1.00 12.17	
ATOM	272	CB	ALA	4.3	55.513	47.145	15.515	1.00 12.56	
ATOM	273	С	ALA	43	57.164	45.291	15.731	1.00 10.70 6	
ATOM	274	0	ALA	43	58.309	45.583	15.930	1.00 13.41	
MOTA	275	N	ALA	44	56.878	44.282	14.903	1.00 3.23 7	
ATOM	276	CA	ALA	44	57.928	43.514	14.208	1.00 3.02 8	
MOTA	277	CB	ALA	44	57.326	42.507	13.263	1.00 4.97 8	
MOTA	278	С	ALA	44	58.828	44.442	13.438	1.00 8.50 6	
MOTA	279	0	ALA	44	58.407	45.534	13.047	1.00 9.57 5	
ATOM	280	N	SER	45	60.086	44.068	13.275	1.00 9.05 7	
MOTA	281	CA	SER	45	60.962	44.925	12.508	1.00 10.31	
ATOM	282	CB	SER	45	61.618	46.002	13.354	1.00 11.34	
MOTA	283	OG	SER	45	61.479	47.244	12.695	1.00 10.35	;
ATOM	284		SER	45	61.996	44.207	11.683	1.00 10.05 3 1.00 13.83 6	;
ATOM	285	0	SEF	45	62.599	43.221	12.124		:
MOTA	286	N	ALA	46	62.113	44.571	10.435	1.00 14.33	:
ATOM	287	CA	ALA	46	63.041	44.134	3.469	1.00 15.72 5 1.00 14.88 7 1.00 14.41 5 1.00 17.21 5	
ATOM	288	CB	ALA	46	52.810	44.781	8.127	1.00 17.01	•
ATOM	289	С	ALA	46	64.379	44.538	10.028		
ATOM	290	9	ALA	46	64.657	45.746	10.203	1.00 15.43	:
ATOM	291	N	GLY	47	55.140	43.525	10.433	1.00 16.67	;
ATOM	292	CA	GLY	47	66.450	43.762		1.00 15.11	
ATOM	293	C	GLY	47	66.558	44.415	11.009	1.00 16.67 3 1.00 15.71 7 1.00 15.77 3	:
ATOM	294	Ö	GLY	47	67.231	44.415	12.400	1.00 15.13	:
ATOM	295	N	VAL	48	65.873	43.843	12.546	1.00 16.53	:
ATOM	296	CA	VA:	48	65.950	44.302	13.399	1.00 13.97	
ATOM	297	CF	VAL	48	64.825	45.230	14.799	1.00 10.23	:
ATOM	298		VAL	48	64.572	45.230	15.231	1.00 8.24 8 1.00 8.06 8	:
ATOM	299	CG2		48	65.21€	45.556	16.701	1.00 8.08	:
ATOM	300	S .	VAL	48	65.904	43.060	14.964		:
ATOM	301	õ	VAL	48	65.062	42.183	15.642	1.00 3.65	
ATOM	302	N	GLY	49	56.882	42.183	15.443	1.00 9.93	•
ATOM	303	CA	GLY	49	66.948	42.949	16.521		
ATOM	304	c.	GLY	49	67.199	42.211	17.393		:
				• •	27,1233	72.21	18.829	1.00 5.14 6	•

bref21	c.pdl	5		Thu	Apr	25 12	: 27:47	1996		5	
ATOM	305	o G	LY	49	6	7.294	43.396	19.152	1.00 3	3.06	5
ATOM			RO	50	6.	7.274	41.234	19.732		1.49	7
ATOM	307	CD P	RO	50		7.104	39.790	19.536		2.00	5
MOTA	308		RO	50		7.519	41.540	21.135		2.99 3.97	5 5
ATOM	309		RO	50		7.545	40.158 39.264	21.762 20. 6 32		2.00	5
ATOM	310		PRO	50 50		7.935 8.837	42.307	21.315	_	4.87	٤
ATOM	311 312		PRO	50		8.962	43.122	22.217		7.36	3
ATOM ATOM	313		SLY	51		9.787	42.100	20.403		5.60	7
ATOM	314		LY	51		1.059	42.792	20.477	1.00	2.83	÷.
ATOM	315		GLY	51	7	0.991	44.263	20.103		3.36	ξ
ATOM	316	0 0	GLY	51		2.025	44.910	19.956		5.85	3
MOTA	317		ASN	52		9.792	44.815	19.968		2.00	ī. 5
MOTA	318		ASN	52		9.670 8.527	46.211 46.401	19.604 18.633		2.00 3.33	ક
MOTA	319		ASN ASN	52 52		8.768	47.534	17.666		7.97	ε
MOTA MOTA	320 321	OD1		52		9.233	47.311	16.538		2.55	ŝ
ATOM	322	ND2		52		8.442	48.753	18.079	1.00 1	0.05	7
ATOM	323		ASN	52	•	9.505	47.144	20.797	1.00	3.59	5
ATOM	324	0	ASN	52	•	59.524	48.359	20.638	1.00	2.00	5
ATOM	325	N '	TYR	53		59.286	46.573	21.985	1.00	5.70	7
ATOM	326		TYP	53		69.148	47.350	23.229	1.00	5.58	ē 5
MOTA	327		TYP	53		67.707	47.412	23.770	1.00	5.70	5
ATOM	328		TYP.	53		66.615	47.547	22.768 22.188	1.00	4.84 6.02	
ATOM	329	CDI		53 53		66.067 65.080	46.414 46.495	21.282	1.00	5.48	5
MOTA	230 331	CE1		53		66.123	48.789	22.405	1.00	5.30	÷
MOTA MOTA	332	CE2		53		65.119	48.891	21.495	1.00	6.56	÷
ATOM	333	CZ	TYP.	53		64.598	47.729	20.929	1.00	8.17	÷
ATOM	334		TYF.	53		63.590	47.767	19.987	1.00		3
MOTA	335	С	TYR	53		69.943	46.667	24.308	1.00	3.83	5
ATOM	336	0	TYR	53		70.176	45.465	24.245	1.00	4.09 3.81	ē 7
MOTA	337	Ŋ	SEP.	54		70.257 70.977	47.428 46.921	25.346 26.501	1.00	6.59	5
MOTA	338	CA	SEP.	54 54		72.296	47.682	26.710	1.00	8.72	ē
ATOM	339 340	CB OG	SER SEP	54		73.405	46.867	26.341	1.00		3
MOTA MOTA	341	C	SER	54		70.077	47.035	27.726	1.00	4.52	5
ATOM	342	0	SER	54		69.495	48.089		1.00	5.58	3
ATOM	343	N	PHE	55		69.931	45.926		1.00	3.52	7
MOTA	344	CA	PHE	55		69.095	45.878		1.00	3.38	é
MOTA	345	CB	PHE	55		68.141			1.00	6.11	÷
ATOM	346	CG	PHE	55		67.052			1.00	6.96	ó
ATOM	347		PHE	55		65.741			1.00	10.17 8.73	é
ATOM	348		PHE	55		67.330 64.713				12.64	
ATOM	349 350		PHE PHE	55 55		66.317			1.00	8.02	ć
ATOM ATOM	351	CZ	PHE	55		65.007			1.00	8.93	÷
ATOM	352		PHE	55		69.942			1.00	2.90	- 5
ATOM	353		PHE	55		70.476		31.200	1.00	2.00	3
ATOM	354		SER	56		70.083	46.892			2.00	-
ATOM	355	CA	SER	56		70.854				5.40	ē
MOTA	356		SER	56		72.159				6.39	÷
ATOM	357		SER	56		71.950				9.05 8.43	5
MOTA	358		SER SER	56 56		70.089				7.21	;
ATOM ATOM	359 360		TYR	57		70.54				7.52	
ATOM	361		TYR	57		69.91				8.61	÷
ATOM	362		TYR	57		69.09	1 45.62	1 36.883	1.00	3.65	÷
ATOM	363		TYR	57		69.86				4.17	á
ATOM	364	CD1	TYR	57		70.25				2.00	- 5
ATOM	365			57		70.86					•
MOTA	366		2 TYR	57		70.11					•
ATOM	36		2 TYR	57 57		70.72					5
MOTA	368		TYR	5.		71.09					:
ATOM	3 6 9 3 7 0		TYR	57		70.88				10.04	4
ATOM ATOM	37		TYR	57		72.09				11.97	
ATOM	37.		GLN	58		70.35				11.03	-
MOTA	37		GLN	58		71.18	1 48.14	3 39.83	2 1.00	9.11	.3
ATOM	37	4 CE	GLN	5 6		71.61				10.64	
ATOM	37			58		72.16				13.28	
MOTA	37			5.6		72.82				13.57	
ATOM	37		1 GLN	56 58		72.16 74.14				15.62 14.36	
ATOM ATOM	37 37		2 GLN GLN	56		70.43					
MOTA	38		GLN	5.8		69.48					
ATOM	38		LEU	5.9		70.7		98 41.76	9 1.00	8.41	
MOTA	38			5 9	÷	70.18	33 46.43	35 43.03	B 1.00	€.43	

bref2	lc.po	i b		Thu	Apr 25	12:27:47	1996		6	
ATOM	383	CB	LEU	59	70.53	4 44.993	43.313	1.00	4.10	•
ATOM	384	CG	LEU	5.9	69.81		44.446			5
ATOM	3 B 5		LEU	59	68.34			1.00	2.46	5
ATOM	386	CD2		59	70.24		44.227	1.00	3.98	5
ATOM	387	C	LEU	59	70.92		44.462	1.00	6.03	6
ATOM	388	Ö	LEU	59	72.13		43.995	1.00	9.36	5
ATOM	389	N	GLU	60	70.22		44.085	1.00	9.93	3
ATOM	390	CA	GLU	60	70.22		44.667		11.94	7
ATOM	391	CB	GLU	60			45.603		13.27	5
					69.85		46.643		14.05	á
ATOM ATOM	392	CC	GLU	60	70.44		47.531		15.91	5
	393	CD	GLU	60	69.44		48.510		16.83	5
ATOM	394	OE1	GLU	60	69.26		49.607		16.52	â
ATOM	395		GLU	60	68.85		48.181		15.77	ŝ
MOTA	396	С	GLU	60	72.15		46.315	1.00	14.73	6
MOTA	397	0	GLU	60	72.20		47.189		14.00	8
ATOM	398	N	ASP	61	73.19		45.973		16.22	7
ATOM	399	CA	ASP	61	74.56		46.452	1.00	17.32	ó
ATOM	400	CB	ASP	61	74.62		47.930	1.00	22.61	5
ATOM	401	CG	ASP	61	74.28		48.814	1.00	26.60	5
MOTA	402		ASP	61	74.28		50.054	1.00	30.15	â
ATOM	403	OD2	ASP	61	74.03		48.271	1.00	27.62	3
ATOM	404	c	ASP	61	75.39		45.610	1.00	16.14	ર્ગ
ATOM	405	0	ASP	61	76.58		45.423	1.00	16.58	3
ATOM	406	N	GLU	62	74.75		45.130	1.00	14.78	7
ATOM	407	CA	GLU	62	75.40	2 46.524	44.223	1.00	13.68	5
MOTA	408	CB	GLU	62	74.41		43.931	1.00	15.90	ક
ATOM	409	CG	GLU	62	74.59	2 44.612	42.585		20.15	ź
MOTA	410	CD	GLU	62	73.57	4 44.998	41.452		18.81	5
ATOM	411	OE1	GLU	62	73.32		41.202		19.09	ā
ATOM	412	OE2	GLU	62	73.04		40.788		17.28	3
ATOM	413	С	GLU	62	75.70		42.947		10.99	ร์
MOTA	414	0	GLU	62	75.06		42.704		11.23	3
ATOM	415	N	PRO	63	76.74		42.173	1.00	9.01	7
MOTA	416	CD	PRO	63	פד.דר		42.435	1.00	9.66	6
MOTA	417	CA	PRO	63	77.06		40.959	1.00	8.47	έ
ATOM	418	CB	PRO	63	78.51		40.691	1.00	5.33	5
MOTA	419	CG	PRO	63	78.50		41.103	1.00	7.09	6
ATOM	420	С	PRO	63	76.14		39.779	1.00		5
ATOM	421	0	PRO	63	75.47		39.775	1.00	6.19 4.91	
ATOM	422	N	TRP	64	76.11		38.788	1.00	3.37	e 7
ATOM	423	CA	TRP	64	75.29		37.613	1.00		
ATOM	424	CR	TPP	64	75.44		36.645		2.00	á
ATOM	425	CG	TRP	64	74.59		26.923	1.00	2.40	5
ATOM	426		TRF	54	73.18			1.00	2.00	5
ATOM	427		TRP	64	72.84		36.678	1.00	2.00	5
MOTA	428		TRP	64	72.17		27.050	1.00	2.28	÷
ATOM	429		TPP	54	75.02	_	36.186	1.00	2.18	÷
ATOM	430	NE1	TRF	54			37.410	1.00	2.00	5
			TRP		73.99		37.487	1.00	2.00	7
ATOM	431		_	64	71.53		36.950	1.00	2.00	÷
ATOM	432	CZ3	TRP	54	70.87		36.087	1.00	2.49	÷
MOTA	433		TRP	64	70.57		35.471	1.00	2.00	6
MOTA	434	С	TP.P	64	75.70		36.903	1.00	2.00	5
MOTA	435	2	TEP	64	76.87		26.736	1.00	2.00	3
ATOM	436	N	LYS	65	74.70		36.524	1.00	2.00	7
ATOM	437	SA	LYS	55	74.90		35.803	1.00	2.00	5
ATOM	438	CB	LYS	55	74.60		26.668	1.00	2.61	
ATOM	439	CG	LYS	6.5	75.61		37.673	1.00	3.35	5
ATOM	440		LYS	6.5	75.20		38.401	1.00	4.33	÷
ATOM	441	CE	LYS	5.5	76.20		39.488	1.00	10.13	ő
ATOM	442	NZ	LYS	65	76.45		40.293	1.00	15.09	7
ATOM	443	C	7.5	55	74.01	7 44.725	24.584	1.00	2.00	5
ATOM	444	Ć.	LYS	55	73.12		34.416	1.00	2.81	3
atom	445	25	LEU	56	74.20	1 43.692	33.780	1.00	2.51	7
ATOM	446	CA	LEU	56	73.42	1 43.532	32.558	1.00	3.38	÷
ATOM	447	ΩВ	LEU	55	74.34		31.340	20	2.07	
MOTA	448	ΦG	LEU	56	75.13		31.138	1.00	2.42	\$ \$ \$ \$ \$ \$
MOTA	449	CD1	LEU	56	76.36		30.416	1.00	5.47	
MOTA	450		LEU	56	74.32		30.383	1.00	2.99	s
ATOM	451	¢	LEU	55	72.65		32.492	1.00	3.16	5
ATCM	452	:	LEU	56	73.12		32.943	1.00	2.56	2
ATOM	453	N	CYS	57	71.47		31.385	1.00		
ATOM	454	CA	CYS	57	70.68		31.708	1.00	4.64	5
ATOM	455	0	CYS	57	70.56		30.191		8.30	
ATOM	456	-5	CYS	57	70.50			1.00	2.34	-5
ATOM	457	DB.	27.2	57	69.33		29.512		11.12	.3
ATOM	453	3 G	CYS	57	58.29		32.363	7.00	9.68	3
ATOM	459	Z	ARG	÷6	70.67		32.300	1.00	9.98	1.5
ATOM	460	CA	AP.G	68	70.5€		29.649 28.187	.00	10.38	
						33.00=	= 0 (10 /	00	11.77	3

bref21	c.pdl	5		Thu .	Apr 25	12:	27:47	1996		7	
ATOM	461	CB A	RG	68	71.3	80 3	38.359	27.627	1.00 15		ŧ.
MOTA	462		RG	68	71.3		38.376	26.053	1.00 2		
ATOM	463	CD A	RG	6B	71.8		37.102	25.359		1.17	<u>-</u>
ATOM	464		RG	68	71.0		35.943	25.653 26.288	1.00 2		Ŧ.
ATOM	465		RG	68 68	71.4 72.7		34.837 34.732	26.705		8.62	-
ATOM	466 467	NH1 A NH2 A	RG RG	68	70.6		33.B18	26.498		7.68	-
ATOM ATOM	468		RG	68.	69.1	.43	39.327	27.751		3.76	÷
ATOM	469		RG	68	68.4		38.504	28.317		9.75	3
ATOM	470		EU.	69	68.7		40.027	26.684		8.16	£
MOTA	471		.EU	69	67.4		39.983	26.131 25.328		5.24 4.64	· •
ATOM	472		EU.	69	67.3 67.4		41.247 42.587	25.980	1.00	5.82	Ē
ATOM	473 474	CG I	EU	69 69	67.		43.727	25.026	1.00	9.48	٤
ATOM ATOM	475	CD2 I		69	66.		42.773	27.111	1.00	9.06	÷
ATOM	476		EU	69	67.2	222	38.794	25.221	1.00	6.45	÷
ATOM	477		LEU	69	68.		38.217	24.655	1.00	6.60	=
ATOM	47B		RIS	70	65.		3B.430	25.133	1.00	6.17	
MOTA	479		HIS	70	65.		37.374	24.296 25.103	1.00	4.34	÷
ATOM	480		HIS HIS	70 70	64. 65.		35.494	25.871	1.00	4.94	÷
ATOM	481 482	CD2 I		70	66.		34.706	25.460	1.00	7.46	÷
ATOM ATOM	483	ND1		70	65.		35.444	27.243	1.00	8.83	-
ATOM	484	CE1		70	66.	738	34.653	27.650	1.00	9.22	<u>:</u>
ATOM	485	NE2	HIS	70		372	34.193	26.586	1.00	6.78	- -
MOTA	486		HIS	70		407	38.097	23.546	1.00	6.62 7.52	
ATOM	487		HIS	70 71		129 871	39.240 37.453	23.863 22.520		20.06	:
ATOM	488		GLN GLN	71		828	36.038	21.676		12.44	ŧ
MOTA ATOM	489 490		GLN	71		449	38.691	20.442		12.64	3
ATOM	491		GLN	71		523	39.628	19.675		12.33	5
ATOM	492		GLN	71		193	40.157	18.423		11.98	÷
ATOM	493	OE1		71		256	41.364	18.185		14.18	ε 7
ATOM	494	NE2		71		741	39.254	17.638 21.278		13.04 14.54	ě
ATOM	495		GLN	71 71		.867 .293	36.915 35.846	20.828		13.15	
ATOM	496 497	N O	GLN ALA	72		.576	37.148	21.510		16.60	5 7
ATOM ATOM	498	ČΆ	ALA	72		.540	36.163	21.222		17.29	5
ATOM	499	CB	ALA	72	59	.106	35.462	22.513		18.25	é
ATOM	500	С	ALA	72		.339	36.816			17.09	é
ATOM	501	O	ALA	72		. 962	37.949			17.99	Ē 7
ATOM	502	N	PRO	73		.770 .266	36.140 34.944			15.70 15.56	÷
MOTA	503 504	CA	PRO PRO	73 73		.618	36.681		1.00	14.26	Ę
atom atom	505		PRO	73		.539	35.789			14.62	÷
ATOM	506		PRO	7.3		.057	34.500			14.52	÷
ATOM	507	C	PRO	73		.392	36.586			13.69	<u> </u>
MOTA	508		PRO	73		. 295	35.678 37.632			16.10 12.65	:
ATOM	509		THP.	74 74		.568	37.789			11.59	<i>f</i>
ATOM	510 511		THR	74		. 987	39.276			3.94	÷
MOTA ATOM	512			74		.100	39.93			12.22	÷
ATOM	513		THR	74	51	.790	39.48			13.10	÷
ATOM	514	C	THR	74		2.216	37.28			13.56	•
MOTA	515		THR	74		2.234	37.63		1.00	15.99 12.64	3
ATOM	516		ALA	75 75		L.237 D.131	36.543 36.07			10.05	
ATOM	517 518		ALA ALA	75		3.995					************
ATOM ATOM	519		ALA	75		9.612			2 1.00	3.70	÷
MOTA	520		ALA	75		9.256			7 1.00	12.33	
ATOM	52		ARG	76		9.583				9.12	
MOTA	52		ARG	76		9.107				10.37	:
MOTA	52.		ARG	76 76		8.870 7.709				10.98 16.38	
ATOM	52		ARG	76		7.936			. i.co	21.72	:
MOTA MOTA	52 52		ARG	76		7.298			7 1.50	23.03	•
ATOM	52		ARG	76		7.700	40.06			25.34	-
MOTA	52	s NHI	1 ARG	76	. 4	8.745			0 1.00	25.68	
ATOM	52	9 NH2	2 ARG	76		7.065				28.25	-
MOTA	53		ARG	76		0.026				12.35 15.69	! <u>-</u>
ATOM	53 53		ARG GLY	70		9.680					-
MOTA MOTA	53 53		GLY	77		2.12				: ::.39	
ATOM	53		GLY	77	5	3.07	9 41.08		9 1.0	10.38	
ATOM	53		GLY	77	5	3.63	3 41.81	4 15.10	2 1.0	10.58	
ATOM	53		ALA	78		3.24				12.04	
MOTA	53			78		4.15					
ATOM	53	8 CB	ALA	78	, :	53.46	5 43.0	41 18.83	252	0.28	

bref21	.c.pd	l b		Thu	Apr 25	12:27:47	1996	8	
ATOM	539	С	ALA	78	55.263	41.329	18.357	1.00 11.11	5
ATOM	540	0	ALA	78	55.080		18.495	1.00 10.01	ŝ
MOTA	541	N	VAL	79	56.418		18.640	1.00 9.69	7
ATOM	542	CA	VAL	79	57.546		19.192	1.00 7.22	5
MOTA	543	CB	VAL	79	58.844	41.391	18.354	1.00 6.05	5
MOTA	544	CG1	VAL	79	58.70€	5 40.741	17.024	1.00 6.29	€
MOTA	545	CG2		79	59.135		18.171	1.00 5.80	ó
MOTA	546	С	VAL	75	57.78€	41.500	20.672	1.00 5.75	ઇ
ATOM	547	0	VAL	79	57.633		21.125	1.00 4.75	3
ATOM	548	N	ARG	80	58.20		21.403	1.00 4.34	7
MOTA	549	CA	ARG	80	58.420		22.813	1.00 7.09	ó
MOTA	550	CB	ARG	80	57.50		23.550	1.00 8.65	3
ATOM	551	CG	ARG	80	57.465		25.052	1.00 7.34	5
ATOM	552	CD	ARG	вс	56.674		25.630	1.00 6.89	
ATOM	553	NE	ARG	80	55.272		25.237	1.00 6.67	
ATOM	554	CZ	ARG	80	54.415		25.313	1.00 4.11	5
ATOM ATOM	555 556	NH1 NH2		80 80	54.829		25.743	1.00 5.04	7
ATOM	557	C	ARG		53.142		25.063	1.00 2.00	
ATOM	558	Ö	ARG	80 80	59.846 60.466		23.297	1.00 5.10	
ATOM	559	N	PHE	81	60.34		23.114	1.00 3.87	
ATOM	560	CA	PHE	81	61.688		23.951	1.00 4.32	
ATOM	561	CB	PHE	91	62.38		24.488	1.00 5.56	
ATOM	562	CG	PHE		62.74		24.305	1.00 4.97	
	563			81			22.915	1.00 5.07	
ATOM ATOM	564	CD1		81 81	61.86		22.091	1.00 6.98	
ATOM	565		PHE	81	63.94		22.409	1.00 7.17	
ATOM	566		PHE	9:	62.164 64.27		20.763	1.00 7.58	
ATOM	567	CZ	PHE	81	63.37		21.086	1.00 10.89	
ATOM	568	C	PHE	81	61.54		20.251 25.955	1.00 10.08	
ATOM	569	0	PHE	81	60.72		26.604	1.00 7.23	
ATOM	570	N	TRP	82	62.30		26.469	1.00 8.68	
ATOM	571	CA	TRP	82	62.26		27.891	1.00 7.82	
ATOM	572	CB	TRP	82	61.25		28.199	1.00 9.85	
ATOM	573	CG	TRP	82	61.58		27.697	1.00 12.09	
ATOM	574		TRP	82	62.23		28.428	1.00 11.52	
ATOM	575		TRP	82	62.32		27.577	1.00 13.27	
ATOM	576		TRF	82	62.74		29.722	1.00 15.01	
ATOM	577	CDI	TRP	32	61.30		26.453	1.00 14.64	
ATOM	578	NE1	TRF	82	61.75		26.378	1.00 12.57	
ATOM	579		TRF	3.2	62.91		27.987	1.00 17.05	
ATOM	580	CZ3		82	63.33		30.137	1.00 16.75	
ATOM	581	CH2	TRE	82	63.41		29.272	1.00 17.82	
ATOM	582	С	TRP	82	63.65		28.371	1.00 8.05	
ATOM	583	0	TRP	82	64.60		27.623	1.00 7.22	
ATOM	584	N	CYS	63	63.76		29.635	1.00 7.16	
ATOM	585	CA	CYS	83	65.02		30.282	1.00 5.52	
ATOM	586	C	CYS	33	64.63	2 38.373	31.702	1.00 4.93	
ATOM	587	0	CYS	88	63.73	7 38.969	32.271	1.00 5.96	5 ē
MOTA	588	CB	CYS	3 3	66.02		30.319	1.00 7.73	5
ATOM	589	SG	CYS	83	66.43		31.992	1.00 15.35	15
ATOM	590	N	SER	34	65.24		22.258	1.00 3.11	7
ATOM	591	CA	SER	84	64.90		33.610	1.00 4.32	2 5
ATOM	592	CB	SEF.	34	64.39		3 3.6 58	1.00 5.70	
ATOM	593	OG	SEP	84	65.09		32.731	1.00 12.40	
ATOM	594	C	SER	34	66.12		34.483	1.00 7.3	
ATOM	595	0	SER	84	67.17		34.190	1.00 11.63	
ATOM		. И	LEU	35	66.00		35.546	1.00 7.6	
MOTA	597	CA	LEU	25	67.11		36.457	1.00 4.8	
ATOM	598	CB	LEU	85	66.67		37.546	1.00 3.5	
ATOM	599	CC	LEU	3.5	66.73		37.197	1.00 5.4	
MOTA	600		LEU	8.5	67.01		38.482	1.00 7.8	
ATOM	601		LEU	3.5	67.84		35.232	1.00 5.4	
ATOM	602	Ş	LEU	3.5	67.70		27.110	1.00 5.0	
ATOM	603	-O	LEU	3.5	67.00		37.352	1.00 9.2	
ATOM	604	N CF:	PRO	36	69.02		37.388	1.00 5.8	
ATOM ATOM	605	CD	PRO	3.5 3.5	69.95		35.989	1.00 5.0	
MOTA	606 607	CA	PRC	3 6 2 4	69.76		38.036	1.00 4.3	
ATOM	608	CB	PRO	86	71.21		37.921	1.00 3.1	
ATOM	609	C	PRC	3 é 3 6	71.20 69.33		35.772	1.00 5.1	
ATOM	610	Ö	PRO	36	69.33 69.14		39.515 40.187	1.00 3.9	
ATOM	611	Ŋ	THR	35	69.22		40.187	1.00 4.2	
ATOM	612	CA	THR	-	68.79		41.394	1.00 5.7	
ATOM	613	CB	THR	87	68.96		41.727	1.00 5.	
MOTA	614		THR	87	68.49		40.607	1.00 9.3	
ATOM	615		THP	ā-	68.14		42.975	1.00 11.5	
MOTA	616	С	THR	s =	69.3		42.531	1.00 7.7	

bref21	c.pdb	Thu Ap	r 25 12:2	27:47 199	6 9
2 TOM	617 O THR	87	68.606 35	5.730 43.38	
ATOM ATOM	618 N ALA	88		5.474 42.54	
ATOM	619 CA ALA	88		6.286 43.56	
ATOM	620 CB ALA	38	_	6.176 43.41	
MOTA	621 C ALA	88		7.752 43.49 8.573 44.24	
MOTA	622 O ALA	98		8.090 42.5°	
MOTA	623 N ASP	9 è.		9.470 42.3	97 1.00 8.96 6
MOTA	624 CA ASP 625 CB ASP	66		9.911 40.9	92 1.00 7.68 5
MOTA	625 CB ASP 626 CG ASP	8 9		9.915 40.7	
atom Atom	627 OD1 ASP	9.9	72.319 4	G.224 41.7	
ATOM	628 OD2 ASP	89		9.646 39.6	
ATOM	629 C ASP	99		9.746 42.6	
MOTA	630 O ASP	89	- '	10.880 42.5 38.724 43.0	· .
ATOM	631 N THP.	90		38.724 43.0 38.866 43.3	
MOTA	632 CA THR	90 90		7.603 42.8	••
MOTA	633 CB THP. 634 OG1 THR	90		36.466 43.4	95 1.00 2.00 B
ATOM	634 OG1 THR 635 CG2 THR	90		37.445 41.4	
ATOM ATOM	636 C THR	90		39.219 44.8	23 1.00 8.87 6
ATOM	637 O THP.	90		38.790 45.3	
MOTA	638 N SER	91		40.043 45.4	
ATOM	639 CA SER	91		40.434 46.8 41.178 47.4	
MOTA	640 CB SER	91		40.343 47.	
ATOM	641 OG SER	91 9:		41.265 47.	
ATOM	642 C SER 643 O SER	91		42.197 46.	
ATOM	643 0 SER 644 N SER	92		41.029 48.	
ATOM	645 CA SER	92	63.000	41.671 48.	
ATOM ATOM	646 CB SER	92	62.022	40.702 49.	
ATOM	647 OG SER	92	61.127	40.120 48.	
ATOM	648 C SER	92	62.732		
ATOM	649 0 SER	92	61.652		744 1.00 10.02 3 764 1.00 5.40 7
ATOM	650 N PHE	93 93	63.600 63.132		366 1.00 3.55 6
ATOM	651 CA PHE	93 93	62.881		879 1.00 2.38 6
MOTA	652 CB PHE 653 CG PHE	93	61.836		207 1.00 2.00 6
MOTA MOTA	653 CG PHE 654 CD1 PHE	93	62.214		444 1.00 2.00 6
MOTA	655 CD2 PHE	93	60.475		232 1.00 2.00 6
ATOM	656 CE1 PHE	93	61.260		689 1.00 2.00 6
MOTA	657 CE2 PHE	93	59.520		.478 1.00 2.00 € .704 1.00 2.00 €
ATOM	658 CZ PHE	93	59.922		.704 1.00 2.00 6 .035 1.00 5.65 6
MOTA	659 C PHE		63.923 €3.753		.657 1.00 5.77 3
ATOM	660 O PHE		64.671		.938 1.00 5.76 7
ATOM	661 N VAI 662 CA VAI		65.542		.410 1.00 4.07 6
atom Atom	663 CB VAI		66.969	46.501 48	.238 1.00 3.20 🐔
ATOM	664 CG1 VAI		67.600		.571 1.00 6.35
ATOM	665 CG2 VA		66.935		.522 1.00 2.00 5
ATOM	666 C VA	, 94	65.042		.040 1.00 6.50 6
MOTA	667 O VA		64.317		.368 1.00 6.26 3
ATOM	668 N PR		65.364		.648 1.00 4.63 7 7.507 1.00 5.07 6
ATOM	669 CD PR		65.947 64.960		3.365 1.00 2.90 5
MOTA	670 CA PR 671 CB PR		65.316		5.530 1.00 2.93 €
ATOM ATOM	671 CB PR 672 CG PR		65.261		7.004 1.00 4.40 €
ATOM	673 C PR		65.783		1.248 1.00 5.07 6 1.399 1.00 7.49 8
ATOM	674 O PR		66.985		1.399 1.00 7.49
ATOM	675 N LE		65.128		3.14100 0.05
ATOM	676 CA LE		65.776		1.957 1.00 5.19 6 1.543 1.00 3.04 6
atom	677 CB LE		65.088 65.571		0.411 1.00 2.00 6
ATOM	676 CG LE		66.945		0.642 1.00 2.00 1
ATOM	679 CD1 LE 680 CD2 LE		64.648		0.315 1.00 2.00
ATOM			65.713		0.816 1.00 6.21 E
ATOM ATOM	1111		64.639	49.309 4	0.367 1.00 5.02 3
ATOM			66.881	49.355 4	0.416 1.00 3.18
ATON			67.000		9.336 1.00 a.49
ATOM		רפ טו	68.315		9.476 1.00 10.17
ATOM	686 CG G	ra 3	68.162		3.849 1.00 10.56
ATOM		רי פיי	67.80		3.676 1.00 12.04 3.734 1.00 14.20
ATOM			68.08° 67.252		7.691 1.30 17.02
7.TO;			66.95		27.987 1.00 8.71
MOTA MOTA		בי טו בי טו	67.73		7.741 1.00 9.01
ATON ATON		EC 38	66.08	-	37.101 1.00 8.76
ATO		EU 98	65.95	4 49.400	35.821 1.00 8.77
ATO		EU 9B	64.59	2 48.695	35.754 1.00 3.21

bref21c.pdb			Thu	Apr 25 1	2:27:47	1996	10	
ATOM	695	CG	LEU	98	64.366	47.487	35.686	1.00 8.97 6
ATOM	696	CD1	LEU	98	62.912	47.080	35.721	1.00 9.15 5
ATOM	697	CD2	LEU	98	65.203	46.309	35.266	1.00 3.89 8
ATOM	698	С	LEU	98	66.141	50.388	34.676	1.00 9.74 5
ATOM	699	0	LEU	98	65.751	51.556	34.781	1.00 11.17 3
ATOM	700	N	ARG	99	66.814	49.945	23.621	1.00 7.82 7
ATOM	701	CA	ARG	99	67.050	50.799	32.467	1.00 8.42 6
ATOM	702 703	CB	ARG	99	68.265	51.701	32.680	1.00 9.99 3
ATOM ATOM	704	CD CD	ARG	99 99	68.319 69.548	52.571	33.915	1.00 13.57 6
ATOM	705	NE	ARG	99	70.798	53.483 52.717	33.832	1.00 15.65
ATOM	706	CZ	ARG	99	71.623	52.634	32.709	1.00 21.42 7 1.00 23.75 6
ATOM	707		ARG	99	71.364	53.271	31.557	1.00 25.09
ATOM	708		ARG	99	72.747	51.921	32.818	1.00 24.11 7
ATOM	709	С	ARG	99	67.294	50.002	31.174	1.00 7.84 5
MOTA	710	0	ARG	99	68.179	49.159	31.118	1.00 8.53 3
ATOM	711	N	VAL	100	66.528	50.307	30.136	1.00 5.56 7
ATOM	712	CA	VAL	100	66.670	49.664	28.852	1.00 5.54 6
ATOM	713	CB	VAL	100	65.321	49.097	28.397	1.00 8.61 6
ATOM	714	CG1	VAL	100	65.446	48.467	27.008	1.00 7.63 6
ATOM	715		VAL	100	64.821	48.100	29.419	1.00 7.70 6
atom atom	716 717	0	VAL VAL	100 100	67.146 66.556	50.745	27.877	1.00 6.61 6
ATOM	718	N	THR	101	68.236	51.831 50.490	27.819 27.156	1.00 3.63 3 1.00 7.98 7
ATOM	719	CA	THE	101	68.768	51.483	25.193	1.00 7.98 7 1.00 10.18 6
ATOM	720	СВ	THP.	101	70.000	52.277	26.748	1.00 8.43 6
ATOM	721	OG1	THP.	101	70.526	51.629	27.908	1.00 13.91
ATOM	722	CG2	THP	101	69.603	53.663	27.148	1.00 11.20 6
atom	723	С	THR	101	69.115	50.926	24.792	1.00 11.66
ATOM	724	0	THR	101	69.483	49.758	24.645	1.00 11.61 8
ATOM	725	N	ALA	102	68.915	51.752	23.767	1.00 12.50 7
ATOM	726	CA	ALA	102	69.216	51.369	22.386	1.00 14.07 5
ATOM	727	СВ	ALA	102	68.735	52.465	21.399	1.00 14.73 5
ATOM ATOM	728 7 29	0	ALA ALA	102 102	70.721 71.511	51.154	22.249	1.00 13.24 6
ATOM	730	N	ALA	103	71.111	51.752 50.332	23.012	1.00 12.22 8
ATOM	731	CA	ALA	103	72.520	50.004	21.270 21.021	1.00 12.73 7 1.00 13.74 6
ATOM	732	CB	ALA	103	72.631	48.712	20.183	1.00 15.06 6
ATOM	733	С	ALA	103	73.250	51.173	20.338	1.00 14.07 5
ATOM	734	0	ALA	103	73.958	51.013	19.345	1.00 16.53 a
ATOM	735	N	SER	104	73.105	52.341	20.931	1.00 12.51 7
ATOM	736	CA	SEP.	104	73.673	53.569	20.440	1.00 10.25
ATOM	737	CB	SEP.	104	72.834	54.066	13.266	1.00 9.41 6
ATOM	738	OG	SER	104	71.434	54.033	19.565	1.00 8.47
ATOM ATOM	739 740	0	SER SEP	104 104	73.507 73.557	54.528	21.600	1.00 11.58 6
ATOM	741	N	GLY	105	73.187	55.746 53.964	21.412	1.00 11.80 E
ATOM	742	CA	GLY	105	73.002	54.747	23.976	1.00 12.64
ATOM	743	С	GLY	105	71.737	55.568	23.980	1.00 13.51 6
ATOM	744	၁	SLY	105	71.507	56.335	24.921	1.00 15.64
MOTA	745	N	ALA	106	70.929	55.433	22.930	1.00 12.54
ATOM	746	CA	ALA	106	69.668	56.166	22.837	1.00 11.65 6
ATOM	747	СВ	ALA	106	69.068	56.040	21.444	1.00 13.77 6
ATOM	748	2	ALA	106	68.752	55.553	23.884	1.00 11.28 6
MOTA MOTA	749 750	O N	ALA PRO	106 107	68.501 68.239	54.338	23.899	1.00 10.70 3
ATOM	751	CD	PRO	107	68.390	56.392 57.855	24.779	1.00 8.60
ATOM	752		PRO	107	67.354	56.019	24.686 25.882	1.00 9.28 6 1.00 7.77 6
ATOM	753	CB	PRC	107	67.282	57.314	25.683	1.00 8.42 6
MOTA	754	CG	PRO	107	67.302	58.358	25.605	1.00 9.15 6
ATOM	755	С	PRO	107	65.964	55.459	25.552	1.00 7.66 4
ATOM	756	0	PRO	107	65.224	56.048	24.781	1.00 8.78 B
ATOM	757	N	ARG	108	65.595	54.353	25.196	
ATOM ATOM	758 759	CA CB	ARG	108	64.290	53.751	25.990	1.00 4.63 5
ATOM	760	CG	ARG ARG	108 108	64.439	52.415	25.288	1.00 7.43
ATOM	761	CD	ARG	108	63.168 62.783	51.903 52.688	24.695 23.460	1.00 10.88 £
MOTA	762	NE	ARG	108	61.461	52.313	22.364	1.00 14.12
ATOM	763	CZ	AP.G	108	61.086	51.084	22.650	1.00 14.12 5 1.00 15.25 1 1.00 15.01 5 1.00 18.31
MOTA	764	NH1	ARG	108	61.917	50.067	22.764	1.00 18.31
MOTA	765		ARG	108	59.858	50.867	22.236	
MOTA	766	C	ARG	108	63.455	53.624	27.253	00 5.36 5
ATOM	767	÷.	AP.G	108	62.420	54.259	27.404	
ATOM ATOM	768 769	N	TYE	109	63.883	52.837	28.263	5.12
ATOM	770	CA CE	TYF. TYR	109 109	63.102		29.509	1.00 5.72
ATOM	771	CG	TYP	109	62.419 61.455	51.350 51.024	29.631 28.544	1.00 7.62
ATOM	772		TYR	109	61.775		27.565	1.10 8.20 8 1.00 11.38 8

bref21	c.pdb	Thu Ap	r 25 12	:27:47		11
ATOM	773 CE1 TYR	109	60.897	49.788		00 12.39
ATOM	774 CD2 TYR	109	60.230	51.642		.00 10.61
ATOM	775 CE2 TYR	109	59.337	51.347		1.00 12.42 f
ATOM	776 CZ TYR	109	59.670	50.421		
ATOM	777 OH TYR	109	58.777	50.152		
MOTA	778 C TYR	109	63.911	52.909		1.00 8.52 5 1.00 9.59 3
ATOM	779 O TYR	109	65.124	52.737	30.794 31.835	1.00 10.99 7
ATOM	780 N HIS	110	63.198	53.259 53.467	33.174	1.00 14.45
ATOM	781 CA HIS	110	63.760 64.468	54.830	33.296	1.00 16.04 6
MOTA	782 CB HIS	110	65.167	55.029		1.00 21.12 6
ATOM	783 CG HIS	110	66.383	54.616	35.04B	1.00 21.71 €
MOTA	784 CD2 HIS	110 110	64.623	55.764	35.652	1.00 24.07 7
ATOM	785 ND1 HIS 786 CE1 HIS	110	65.476	55.803	36.662	1.00 23.40 6
ATOM	786 CE1 HIS 787 NE2 HIS	110	66.553	55.114	36.321	1.00 22.60 7
MOTA MOTA	788 C HIS	110	62.628	53.380	34.214	1.00 12.21 6
ATOM	789 0 HIS	110	61.740	54.224	34.240	1.00 13.06 8 1.00 11.08 7
ATOM	790 N ARG	111	62.693	52.361	35.062	
ATOM	791 CA ARG	111	61.716	52.116	36.112	
ATOM	792 CB ARG	111	60.878	50.881	35.742	
ATOM	793 CG ARG	111	59.700	50.590	36.641 35.862	1.00 8.05 5 1.00 8.40 5
MOTA	794 CD ARG	111	58.370	50.465	35.783	1.00 8.93 7
MOTA	795 NE ARG	111	57.828	49.099 48.521	36.730	1.00 8.80
ATOM	796 CZ ARG	111	57.096 56.822	49.182	37.840	1.00 10.13 7
MOTA	797 NH1 ARG	111	56.585	47.308	36.550	1.00 10.84 7
MOTA	798 NH2 ARG	111	62.546		37.369	1.00 11.27 8
MOTA	799 C ARG 800 G ARG	111 111	63.776	_	27.306	1.00 13.11 3
MOTA	800 O ARG 801 N VAL	112	61.877		38.510	1.00 11.56 7
MOTA	802 CA VAL	112	62.493	51.471		1.00 11.15 6
MOTA MOTA	803 CB VAL	112	6 2.88 2			1.00 12.50 6
ATOM	804 CG1 VAL	112	63.003			1.00 13.08 6
ATOM	805 CG2 VAL	112	64.235			
ATOM	806 C VAL	112	61.398			1.00 7.77 5 1.00 8.50 3
ATOM	807 0 VAL		60.266			1.00 5.20 7
ATOM	808 N ILE		61.709			1.00 6.80 6
ATOM	809 CA ILE		60.692			1.00 5.60 6
ATOM	810 CB ILE		60.223			1.00 6.45 6
MOTA	811 CG2 ILE		59.680 61.390			1.00 7.39 5
MOTA	812 CG1 ILE	_	61.01			1.00 9.87 6
ATOM	813 CD1 ILE 814 C ILE		61.10			1.00 7.16 6
ATOM			62.14			1.00 9.02 €
ATOM	815 C ILE 816 N HIS		60.26		0 43.463	1.00 2.78 7
MOTA MOTA	817 CA HIS		60.50	3 46.18		1.00 2.00 5
ATOM	818 CB HI		59.79	3 46.75		
ATOM	819 CG HI		60.55			1.00 2.00 5
ATOM	620 CD2 HI	\$ 114	61.33			
ATOM	821 ND1 HI		60.58			
ATOM	822 CE1 HI		61.36			
ATOM	823 NE2 HI		61.83			
ATOM	824 C HI		59.90 58.70			
MOTA	825 O HI		60.74			
ATOM	826 N IL 827 CA IL		60.2			1 1.00 2.00 5
MOTA	827 CA IL 828 CB IL		61.4			3 1.00 3.84 &
ATOM	829 CG2 II		60.9		43.984	
ATOM ATOM	830 · CG1 II	_	62.3			0 1.00 2.00 5
ATOM	831 CD1 II		63.7			6 1.00 2.23 6
ATOM		E 115	59.1			
ATOM		E 115	58.2			
ATOM	834 N A	SN 116	59.0			
ATOM	835 CA A	SN 116	57.9			
MOTA	836 CB A	SN 116	58.3		_	
ATOM		SN 116	58.5		_	
MOTA			59.4 57.8			
ATOM			56.5			
ATOM	_	SN 116 SN 116	55.3			
ATOM	_	LU 117	56.6	_		11 1.00 8.36
MOTA MOTA	·	LU 117	55.4			36 1.00 7.65
ATOM		LU 117	55.	732 46.1		
ATOM		LU 117	55.9			
ATO	4 946 CD G	LC 117	56.			
ATO	M 847 OE1 G		56.			
ATO			55.			
ATO		LU 117	55. 54.			
ATO	м 350 э с	117	34.	4J.		

bref21	c.pc	i b		Thu	Apr 25 12	2:27:47	1996	12	
ATOM	851	N	VAL	118	55.477	43.151	43.523	1.00 3.55	7
ATOM	852	CA	VAL	118	55.226	42.839	42.137	1.00 2.91	•
ATOM	853	CB	VAL	118	56.373	43.488	41.261	1.00 2.00	Ī
ATOM	854	CG1	VAL	118	57.484	42.519	40.942	1.00 2.85	٤
MOTA	855	CG2		118	55.828	44.165	40.062	1.00 2.00	÷
MOTA	856	С	VAL	118	55.060	41.334	41.948	1.00 2.18	ŧ
ATOM	B57	0	VAL	118	55.453	40.755	40.936	1.00 3.50	3
ATOM	B58	N	VAL	119	54.404	40.716	42.919	1.00 2.79	-
ATOM	859	CA	VAL	119	54.155	39.276	42.896	1.00 3.05	:
ATOM	860	CB CG1	VAL	119	53.778	38.736	44.305		=
ATOM ATOM	861 862	CG2		119 119	53.749 54.735	37.267	44.292		÷
ATOM	863	C	VAL	119	52.998	39.231 38.960	45.352 41.945		÷
ATOM	864	õ	VAL	119	52.007	39.674	41.932		£
ATOM	865	N	LEU	120	53.171	37,919	41.132		-
MOTA	866	CA	LEU	120	52.175	37.411	40.174		é
ATOM	867	CB	LEU	120	52.446	37.894	38.745		ś
MOTA	868	CG	LEU	120	51.496	37.332	37.674		5
ATOM	869		LEU	120	50.125	37.938	37.790	1.00 9.95	5
ATOM	870	CD2		120	52.053	37.605	36.306		5
ATOM ATOM	871 872	0	LEU LEU	120	52.289	35.887	40.262		5
ATOM	873	N	LEU	120 121	52.985 51.600	35.241 35.340	39.487	1.00 2.00	ė
ATOM	874	CA	LEU	121	51.629	33.340	41.250 41.552		-
ATOM	875	CB	LEU	121	51.063	33.689	42.964	1.00 2.77 1.00 4.57	£ .
ATOM	876	CG	LEU	121	52.050	33.227	44.062	1.00 10.24	ž Š
ATOM	877	CD1		121	52.939	32.076	43.550	1.00 14.57	:
ATOM	878	CD2		121	52.944	34.328	44.501	1.00 9.45	÷
ATOM	879	С	LEU	121	50.974	32.995	40.554	1.00 5.41	
ATOM	880	0	LEU	121	50.256	33.420	39.654	1.00 7.90	3
ATOM	881	N	ASF	122	51.279	31.709	40.672	1.00 8.57	7
ATOM	882	CA	ASP	122	50 .68 7	30.726	39.782	1.00 6.90	ć
ATOM	883	CB	ASP	122	51.493	29.421	39.773	1.00 7.76	5
ATOM ATOM	884 885	CG	ASF	122	52.701	29.437	38.795	1.00 9.54	á
ATOM	886		ASP ASP	122 122	52.927 53.411	30.429	38.066	1.00 9.98	5
ATOM	887	C	ASP	122	49.292	28.405 30.494	38.748	1.00 10.20	3
ATOM	888	Ö	ASP	122	48.957	30.954	40.343	1.00 7.04 1.00 5.44	5 E
ATOM	889	N	ALA	123	48.464	29.813	29.568	1.00 6.22	7
ATOM	890	CA	ALA	123	47.107	29.562	40.010	1.00 4.76	5
ATOM	891	CB	ALA	123	46.187	29.374	38.839	1.00 2.00	÷
ATOM	892	C	ALA	123	46.981	28.398	40.954	1.00 3.93	÷
ATOM	893	0	ALA	123	47.826	27.484	40.971	1.00 5.37	Ē
MOTA	894	N	PRO	124	45.979	28.490	41.846	1.00 2.51	7
ATOM	895	CD	PRO	124	45.216	29.736	42.096	1.00 2.90	÷
ATOM	896	CA	PRO	124	45.652	27.478	42.845	1.00 2.91	÷
ATOM ATOM	897 898	CB CG	PRO PRO	124 124	44.362	28.022	43.436	1.00 2.00	÷
ATOM	899	c	PRO	124	44.602 45.451	29.485 26.111	43.432	1.00 2.00	•
ATOM	900	ō	PRO	124	45.289	26.022	42.172	1.00 2.00 1.00 2.00	÷
ATOM	901	N	VAL	125	45.524	25.042	42.944	1.00 2.31	-
ATOM	902	CA	VAL	125	45.345	23.715	42.381	1.00 4.06	÷
ATOM	903	CB	VAL	125	46.724	23.006	42.025	1.00 2.00	÷
MOTA	904		VAL	125	47.474	23.806	40.974	1.00 2.33	÷
ATOM	905		VAL	125	47.584	22.776	43.256	1.00 2.03	Ē
ATOM	906	Č	VAL	125	44.436	22.838	43.267	1.00 5.51	:
ATOM	907	0	VAL	125	44.002	23.281	44.316	1.00 6.33	1 5
ATOM ATOM	908		GLY	126	44.068	21.661	42.768	1.00 5.23	-
ATOM	909 910	CA C	GLY	126 12€	43.230 41.939	20.735 21.283	43.494	1.00 4.13	
ATOM	911	Ö	SLY	126	41.588	20.981	45.170	1.00 5.56 1.00 8.97	=
ATOM	912	N	LEU	127	41.248	22.113	43.268	1.00 5.83	-
ATOM	913	CA	LEU	127	39.971	22.667	43.718	1.00 7.8	:
ATOM	914	CB	LEU	12-	39.594	23.949	42.935	1.00 9.72	:
ATOM	915	CG	LEU	12-	38.175	24.573	43.071	1.00 11.04	1
MOTA	916		LEU	12~	37.954	25.322	44.424	1.00 7.43	÷
ATOM	917		LEU	127	37.942	25.516	41.892	1.00 10.21	:
ATOM	918	C	LEU	12	38.846	21.523	43.612	1.00 6.98	:
ATOM	919	0	LEC	12-	38.585	21.083	42.53B	1.00 6.56	•
ATOM ATOM	920 921	N C	VAL	128	38.177	21.369	44.737	1.00 7.11	•
ATOM	921	CA CB	VAL VAL	128 128	37.087 37.485	20.406	44.815	1.00 6.92	:
ATOM	923		VAL	128	37.465	19.147 18.080	45.616	1.00 7.07 1.00 7.35	÷
ATOM	924		VAL	128	38.521	19.477	46.659	1.00 7.35 1.00 9.51	•
ATOM	925	Ç	VAL	128	35.862	21.001	45.470	1.00 5.17	:
ATOM	926	0	VAL	128	35.973	21.795	45.374	1.00 6.97	÷
ATOM	927	N	ALA	129	34.691	20.574	45.031	1.00 7.13	:
ATOM	928	CA.	ALA	129	33.430	21.061	45.579	1.00 6.61	÷

bref21	c.pdl	ь		Thu	Apr	25	12	:27:4	7 1	996	13	3
ATOM	929	СВ	ALA	129	3	2.58	5	21.680			.00 4.36	
ATOM	930	С	ALA	129		2.69		19.876			1.00 9.11 1.00 9.32	
ATOM	931		ALA	129		32.73		18.760			1.00 9.32 1.00 9.70	
MOTA	932	N	ARG	130		32.01 31.28		20.106			1.00 10.5	
ATOM	933	CA	ARG	130 130		32.22		18.310			1.00 11.8	_
MOTA	934	CB	ARG ARG	130		31.76		16.979			1.00 11.8	7 - ნ
ATOM	935 936	CD	ARG	130		32.10		16.871			1.00 15.6	
atom atom	937	NE	ARG	130	;	33.3	51	17.567			1.00 15.7	
ATOM	938	CZ	ARG	130	:	33.6	69	18.135		.414	1.00 20.4	_
ATOM	939	NH1	ARG	130		32.8		18.092			1.00 18.0	
ATOM	940	NH2	ARG	130		34.8		18.791			1.00 21.0	-
MOTA	941	С	ARG	130		30.0		19.479		3.721 9.250	1.00 10.7	
ATOM	942	0	ARG	130		29.9 29.0		18.582		3.792	1.00 12.0	
ATOM	943	N	LEU LEU	131 131		27.B		18.909		9.460	1.00 13.6	
ATOM	944 945	CA CB	LEU	131		26.6		18.313		8.688	1.00 12.7	
ATOM ATOM	946	CG	LEU	131		25.3		18.51		9.353	1.00 11.9	
ATOM	947		LEU	131		25.0	35	20.002		9.487	1.00 10.4	
ATOM	948		LEU	131		24.2		17.78		8.531	1.00 11.6	
ATOM	949	С	LEU	131		27.7		18.40		0.892	1.00 13.4	
ATOM	950	0	LEU	131		27.7		17.20		1.128 1.834	1.00 12.8	
ATOM	951	N	ALA	132		27.9		19.32		3.249	1.00 16.2	
ATOM	952	CA	ALA	132		27.9		20.22		4.122	1.00 14.	
MOTA	953	CB	ALA	132 132		26.6		18.32		3.656	1.00 16.	
ATOM	954 955	0	ALA ALA	132		25.		19.00		4.109	1.00 16.	9 7 ŝ
ATOM ATOM	956	N	ASP	133		26.		17.00		3.411	1.00 20.	
ATOM	957	CA	ASP	133		25.3	397	16.15		3.729	1.00 22.	_
ATOM	958	CB	ASP	133		25.1		14.75	-	4.193	1.00 23.	
MOTA	959	CG	ASP	133		26.		12.78		3.024	1.00 25.	
ATOM	960		L ASP	133		25.		14.01		31.871	1.00 26.	
MOTA	961		2 ASP	133		26.		12.75		4.885	1.00 22.	
MOTA	962		ASP	133		24.	5 75	17.43		54.715	1.00 24.	_
ATOM	963		ASP	133 134			310			56.037	1.00 19.	
ATOM	964		GLU	134			742			57.211	1.00 18.	
MOTA	965 966		GLU	134			478			58.482	1.00 17.	
MOTA MOTA	967			134			589		97 :	58.287	1.00 17.	
ATOM	968			134		28.	003			58.153	1.00 20.	
ATOM	969	OE	1 GLU	134			980			58.020	1.00 19.	
ATOM	970		2 GLU	134			136			58.183 57.068	1.00 18.	
MOTA	971		GLU	134			784	_		57.197	1.00 18	
MOTA	972		GLU SER	134 135			. 842 . 648			56.657	1.00 16	
ATOM	97: 97:						. 375			56.510	1.00 17	.66 5
MOTA MOTA	97						. 435			57.166	1.00 17	
ATOM	97					25.	. 623			55.400		
ATOM	97		SER	135	5		. 99			55.124		
ATOM	97	8 0	SEP				.36			54.991		
ATOM	97		GLY				.28			54.095		
MOTA	98						. 94		.09	52.753 52.372		
MOTA	98		GLY				.76			51.910		
ATOM	98		GL) HIS				.07			52.622		
ATOM ATOM	98 98						.99			52.301		.69 -
ATOM	98						.59		884	53.590		
ATOM	98					25	.76			54.204		
ATOM	98		D2 HI	5 13	7		. 04			55.183		
ATOM	98		DI HI				. 48			53.77		
ATOM	98	_	El HI				.01			54.469		
MOTA	99		E2 HI				1.94			51.32		
ATOM	99						7.08 7.42			51.30		
MOTA	99						7.54			50.46		
ATOM ATOM		93 N 94 C	AV A				8.59			49.52		
ATOM			в ул				8.3		107	48.14		
ATOM			G1 VA			2	9.72	25 24.	286	47.39		
MOTA			G2 VA	L 13	85		7.4		258	47.29		
ATOM	9	98 (. VA	L 13	38		9.8		377	50.15		
. ATOM			V.		38		9.9		376	50.70		9.36
ATOM	10		V.		39		0.8		. 98 2 . 26 9	50.17 50.72		
ATOM	10		CA VA		39 36		2.1		371	51.94		5.78
MOTA	10		CB VA		39 36		3.7		877	52.62		7.80
ATOM ATOM			CG1 VA		39 39		1.4		.393	52.94		6.80
ATOM			CGZ VI		39		3.2		.095	49.63		
ATOM					39		3.3		.026	43.9		

bref2	lc.pd	ъ		Thu	Apr 25 1	.2:27:47	1996		14	
ATOM	1007	N	LEU	140	33.975	24.194	49.372	1.00	a.25	7
MOTA	1008	CA	LEU	140	35.027	24.306	43.384	1.00	6.26	ė
ATOM	1009	CB	LEU	140	34.986	25.673	47.761	1.00	2.05	÷
ATOM	1010	CG	LEU	140	33.726	25.968	47.000	1.00	2.00	ś
ATOM	1011	CD1	LEU	140	33.806	27.395	46.505	1.00	2.00	5
ATOM	1012	CD2	LEU	140	33.594	24.972	45.869	1.00	2.00	6
ATOM	1013	С	LEU	140	36.354	24.170	49.069	1.00	3.88	દ
MOTA	1014	0	LEU	140	36.566	24.774	50.115	1.00	10.60	ŧ
atom	1015	74	ARG	141	37.278	23.481	48.409	1.00	11.34	7
MOTA	1016	CA	ARG	141	38.618	23.235	48.929	1.00	12.76	చ్
ATOM	1017	CB	ARG	141	38.682	21.805	49.446		16.99	6
ATOM	1018	CG	ARG	141	39.347	21.645	50.793		21.35	5
ATOM	1019	CD	ARG	141	40.849	21.410	50.697		24.13	6
ATOM	1020 1021	NE CZ	ARG	141	41.431	21.433	52.042		29.12	7
ATOM ATOM	1021		ARG ARG	141 141	42.344 42.821	22.314 23.266	52.482 51.673		30.00	5 7
ATOM	1023		ARG	141	42.727	22.282	53.773		30.75 29.95	,
ATOM	1024	C	ARG	141	39.632	23.383	47.804		13.10	6
ATOM	1025	ŏ	ARG	141	39.289	23.227	46.639		13.55	3
ATOM	1026	N	TRP	142	40.871	23.715	48.154		11.10	7
ATOM	1027	CA	TRP	142	41.941	23.846	47.182	1.00	6.61	5
ATOM	1028	CB	TRP	142	41.754	25.107	46.354	1.00	6.92	5
ATOM	1029	CG	TRP	142	41.661	26.356	47.155	1.00	9.55	5
ATOM	1030	CD2	TPP	142	40.482	26.905	47.749	1.00	9.85	é
ATOM	1031	CE2	TRP	142	40.852	28.094	48.397	1.00	9.31	5
MOTA	1032	CE3	TRP	142	39.145	26.508	47.788	1.00	10.67	5
ATOM	1033	CD1	TRF	142	42.671	27.216	47.456		10.90	ē.
ATOM	1034	NE1	TRP	142	42.196	28.267	48.209	1.00	11.52	÷
ATOM	1035	CZ2	TRP	142	39.937	28.885	49.072		11.31	5
ATOM	1036	CZ3	TRP	142	38.245	27.296	43.454	1.00	11.65	5
ATOM	1037		TRP	142	38.645	28.474	49.089	1.00	9.80	5
ATOM	1038	С	TRP	142	43.288		47.877	1.00	5.00	6
ATOM	1039	0	TRP	142	43.380		49.076	1.00	6.66	3
MOTA	1040	N	LEU	143	44.349		47.109	1.00	5.47	7
ATOM	1041	CA	LEU	143	45.700		47.656	1.00	3.56	6
ATOM	1042	CB	LEU	143	46.520		47.123	1.00	2.35	5
ATOM	1043	CG	LEU	143	46.031		47.408	1.00	2.00	6
ATOM	1044		LEU	143	46.832		46.601	1.00	2.00	6
ATOM ATOM	1045 1046	CDZ	LEU	143 143	46.182		48.862	1.00	2.00	é
ATOM	1047	0	LEU	143	46.310 45.765		47.158	1.00	2.00	5
ATOM	1049	N	PRO	144	47.411		46.274	1.00	4.81	ŝ 7
ATOM	1049	CD	PRO	144	48.003		47.762 49.030	1.00	2.00	
ATOM	1050	CA	PRO	144	48.027		47.295	1.00	2.00 2.00	÷
ATOM	1051	CB	PRO	144	48.955		43.445	1.00	2.00	5
ATOM	1052	CG	PRO	144	48.442		49.601	1.00	2.00	÷
ATOM	1053	c	PRO	144	48.821		46.011	1.00	2.00	4
ATOM	1054	Ċ.	PRO	144	48.999		45.580	1.00	2.00	3
ATOM	1055	N	PRO	145	49.249		45.342	1.00	2.00	7
ATOM	1056	CD	PRO	145	49.058		45.645	1.00	2.00	ž
ATOM	1057	CA	PRO	145	50.022		44.113	1.00	2.72	4
MOTA	1058	CB	PRO	145	50.532		43.839	1.00	2.80	5
ATOM	1059	CG	PRO	145	49.467	29.898	44.372	1.00	2.95	5
MOTA	1060	С	PRO	145	51.178	26.696	44.455	1.00	4.71	÷
MOTA	1061	0	PRO	145	51.87		45.448	1.00	3.80	<u> </u>
MOTA	1062	N	PRO	146	51.39		43.639	1.00	3.22	
MOTA	1063	CD	PRO	146	50.738		42.347	90	5.90	÷
ATOM	1064		PRO	146	52.462		43.857	1.00	6.83	<u>.</u>
ATOM	1065	CB	PRO	146	52.358		42.622	1.00	7.88	
ATOM	1066	CC	PRO	146	50.97		42.167	1.00		÷
ATOM ATOM	10,67	ث م	PRO	146	53.863		43.967	1.00		÷
ATOM	1068		PRO	146	54.272 54.60		43.135		10.56	3
ATOM	1069 1070	N	GLU	147	55.95		44.975 45.248	1.00		;
ATOM	1070	CA	GLU GLU	147	56.89		44.077	1.00		é E
ATOM	1072	CC	GTf.	147	56.73		43.456		9.95 18.10	
ATOM	1073	CD	GLU	147	57.47		44.166		22.76	÷ ÷
ATOM	1074	SE:		147	58.33		45.061		25.12	÷
ATOM	1075		GLU	147	57.20		43.789		23.73	3
ATOM	1076	5	GLU	147	56.05		45.624	1.00	10.12	*
ATOM	1077	5	GLU	147	57.09		45.453		12.66	4
ATOM	1078	N	THR	148	54.97		45.124	1.00	10.44	7
ATOM	1079	CA	THE	148	55.04		46.541	1.00	7.07	:
ATOM	1080	CB	THE	148	53.77		45.178	_ 00	5.61	•
ATOM	1081		THR.	148	53.58		44.765	1.00	4.74	3
ATOM	1082		2 THE	148	53.88		45.621	1.00		÷
ATOM	1083	C	THR	148	55.27		43.048	50		- 5
MOTA	1084	O	THR	146	54.60	9 28.080	43.789	1.00	4.53	i

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ATOM	1085	N	PRO	149		56.279		. 605	48.503 47.666	1.00	7.63 4.62		
ATOM	1086	CD	PRO	149		57.156 56.623		.457 .757	49.926	1.00	5.20	£	
MOTA	1087	CA	PRO	149 149		58.074		.190	49.860	1.00	2.62		
MOTA	1088	CB CG	PRO PRO	149		58.050		.144	48.69B	1.00		6	
ATOM	1089 1090	C	PRO	149		55.742		.869	50.498	1.00	7.00		
ATOM ATOM	1091	Õ	PRO	149		55.080		.600	49.737		10.83		
MOTA	1092	N	MET	150		55.727		.012	51.814	1.00			
ATOM	1093	CA	MET	150		54.916 55.415		.469	52.109	1.00		5 - 5	
ATOM	1094	CB	MET MET	150 150		56.864		.812	52.512	1.00) :	
ATOM ATOM	1095 1096	SD	MET	150		57.164	33	.978	54.292	1.00			
ATOM	1097	CE	MET	150		57.009		.706	54.546	1.00			
ATOM	1098	С	MET	150		53.411		1.927 2.952	52.169 52.002	1.00			
MOTA	1099	0	MET	150		52.745 52.87		0.696	52.239	1.00			
ATOM	1100	N CA	THR THR	151 151		51.46		0.405	51.963	1.00	3.5		
ATOM	1101 1102	CB	THR	151		51.15	7 21	B.902	51.799	1.00			
ATOM ATOM	1103		THR	151		51.58		8.183	52.955	1.0			
ATOM	1104	CG2	THR	151		51.82		8.347 0.920	50.609 52.922	1.0			•
MOTA	1105	C	THR	151 151		50.40 49.21		0.919	52.583	1.0			
ATOM	1106	0	THP. SER	152		50.77		1.331	54.123	1.0			
MOTA	1107 1108	N CA	SER	152		49.75		1.831	55.041	1.0			<u> </u>
MOTA MOTA	1109	CB	SER	152		50.17		1.598	56.476	1.0	0 6.4		{
ATOM	1110		SER	152		51.02		2.645	56.893		0 5.3	. 8	9 5
ATOM	1111	C	SER	152		49.56	_	3.321	54.842 55.687				2
MOTA	1112		SER	152		48.98		13.976 13.866	53.780		0 7.2	23	-
MOTA	1113		HIS	153		50.14 50.0		35.291	53.485			69	Ę
MOTA	1114			153		51.4		35.883					ē.
ATOM	1115			153 153		52.3		35.975			0 4-		E
MOTA MOTA	1116		2 HIS	153		52.8		37.048	55.183				£
ATOM	1116		1 HIS	153		52.7		34.868					7
ATOM	1119		1 HIS	153		53.5		35.254				00	5
ATOM	1120		2 HIS	153		53.5		36.570				54	5
MOTA	112		HIS	153		49.2 49.0		35.491 36.614				78	ŝ
MOTA	112		HIS			48.9		34.38			_	00	7
ATOM	112		ILE A ILE	_		48.2		34.41				00	÷
MOTA MOTA	112 112					48.4		33.11				CO	÷
ATOM	112		G2 ILE			47.9		33.20				06	
MOTA	112	7 C	G1 ILE			49.9		32.88				.00	ŧ
ATOM	112		D1 ILE			50.3 46.7		31.72				.05	•
ATOM	112					46.1		33.89				.00	:
MOTA	_					46.0		35.39				.56	
MOTA MOTA			A AR			44.	638	35.64				.20	:
ATOM		-	B AR		5	44.		37.14				.20	ē
ATOM	_		G AR			44.		37.92	_		.00 8 .00 14	.42	ě
ATOM			D AR			44.		39.39			.00 24		-
ATOM			E AR		55	44.	832	41.22		96 1	.00 27	. 35	÷
ATOM		_	CZ AR NH1 AR		55 55		718	41.84		99 :	.00 25	. 45	•
MOTA MOTA			NH2 AR		55		600	41.70			.00 28		
4OTA			C AR		55		067	34.9					•
ATON			O AR		55		800	34.7				.12	3
ATOR	M 11		N TY		56		783	34.5				. 24	
ATO			CA TY		56 56		774	32.4				5.18	:
ATO			CB TY		56		978	31.6		39 :	00 10).55	
ATO			CD1 T		56		.447	31.5		551	20 13	3.∔9	:
ATO ATO			CE1 T		56	44	. 624	30.8		968	00 1	6.29	
ATO	_	48	CD2 T		56		.700	31.0		341	.00 1		÷
ATO		49	CE2 T		.56		.899	30.2		546		4.32	-
OTA		50			.56		.346	30.2		360	1.00 1 1.00 1	2.25	•
ATO		51			56		.495	29.5 34.6				7.25	;
ATO		152			156 156		.153			256	1.50	8.19	3
ATO		153			157		.286			107	1.00	4.99	
ATC ATC		154 155			157		.979		38 45.	720	1.00	4.80	
ATC		156			157	39	.036	36.2			1.00	4.31	
ATO		157	CG G	LU	157		. 632			614	1.::	3.5	
ATC	OM 1	158			157		.577			726 232	1.00	2.35	
ATC		159	OE1 G		157		1.568 1.486			514	1.00	5.11	
ATO		160	OE2 G		157 157		3.254			997	1.00	6.09	
TA TA		161 162			157		799			102	1.00		
		_											

bref2	lc.po	iь		Thu	Apr 25	12:27:47	1996		16	
ATOM	1163	N	VAL	158	37.022	33.675	45.406	1.00	5.40	7
ATOM	1164	CA	VAL	158	36.196		44.842	1.00	6.15	ŧ
ATOM	1165	CB	VAL	158	35.459		45.954	1.00	3.03	÷
ATOM	1166		VAL	158	34.655		45.391	1.00	4.03	
ATOM ATOM	1167		VAL	158	36.429		46.962	1.00	3.63	÷
ATOM	1168 1169	0	VAL VAL	158 158	35.154 34.400		43.878	1.00	9.07	ક
ATOM	1170	N.	ASP	159	35.114		44.208		10.93	9 7
ATOM	1171	CA	ASP	159	34.147		41.672		10.57	
ATOM	1172	CB	ASP	159	34.828		40.327		11.17	÷
ATOM	1173	CG	ASP	159	33.873		39.256	1.00 1		ş
ATOM	1174	OD1	ASP	159	33.863		38.172		3.65	3
ATOM	1175		ASP	159	33.093	34.407	39.547	1.00 1	5.65	÷
ATOM	1176	С	ASP	159	32.997		41.575	1.00	9.91	5
ATOM	1177	0	ASP	159	33.227		41.474		1.09	= -
ATOM ATOM	1178 1179	N CA	VAL VAL	160	31.766		41.637	1.00	7.B3	
ATOM	1180	CB	VAL	160 160	30.582 29.637		41.535	1.00	5.49	6
ATOM	1181		VAL	160	28.512		42.755 42.742	1.00	3.19	÷
ATOM	1182		VAL	160	30.362		44.091	1.00	3.00	5 5
ATOM	1183	С	VAL	160	29.842		40.286	1.00	6.19	5
ATOM	1184	0	VAL	160	29.364		40.238	1.00	8.22	•
ATOM	1185	N	SER	161	29.835	31.272	39.300	1.00	7.72	7
ATOM	1186	CA	SER	161	29.104		38.046	1.00	8.29	é
ATOM	1187	CB	SER	161	30.094		36.891	1.00]		•
ATOM ATOM	1188 1189	OG C	SER SER	161	30.637		26.934		3.94	÷
ATOM	1190	0	SER	161 161	28.161 28.601		37.938	1.00	7.24	é
ATOM	1191	N	ALA	162	26.885		38.024 37.791	1.00	7.94	7
ATOM	1192	CA	ALA	162	25.793		27.784	1.00	9.16	=
ATOM	1193	CB	ALA	162	24.689		38.736	1.00		5
ATOM	1194	С	ALA	162	25.199		36.379	1.00		
ATOM	1195	0	ALA	162	25.593		35.406	1.00 1		÷
ATOM	1196	N	GLY	163	24.220	28.499	36.369	1.00 1		7
ATOM	1197	CA	GLY	163	23.598		35.150	1.00 1	6.65	5
ATOM	1198	С	GLY	163	22.561		34.370	1.00-1		5
ATOM	1199	0	GLY	163	21.996		34.897	1.00 1	8.80	3
ATOM ATOM	1200	N	ASN	164	22.416		33.146		90.00	7
ATOM	1201 1202	CA CB	ASN ASN	164 164	21.568 20.505		31.994	1.00		Ę
ATOM	1203	CG	ASN	164	19.337		31.685 32.702	1.00 9	90.00	÷
ATOM	1204		ASN	164	19.322		33.726	1.00		6
ATOM	1205		ASN	164	18.334		32.511		90.00	7
ATOM	1206	С	ASN	164	20.728		32.186		90.00	5
ATOM	1207	၁	ASN	164	19.665		32.817		90.00	
ATOM	1208	N	GLY	165	21.227		31.601	1.00 9	90.00	3 7
ATOM	1209	CA	GLY	155	20.544		31.514		90.00	÷
ATOM ATOM	1210	0	GLY	165	20.274		32.859	1.00		÷
ATOM	1212	О И	GLY ALA	165 166	19.470 20.941		32.927		90.00	=
ATOM	1213	CA	ALA	166	20.602		33.967 35.242		90.00	
ATOM	1214	CB	ALA	166	19.550		35.242	1.00		÷
ATOM	1215	c	ALA	166	21.795		36.188	1.00		5
ATOM	1216	Ó	ALA	166	21.646		37.421	1.00		3
ATOM	1217	N	GLY	167	22.964		35.614	1.00		7
ATOM	1218	CA	GLY	167	24.167	34.185	36.400	1.00		5
MOTA	1219	C	GLY	157	24.110		35.704	1.00		5
ATOM		. 0	GLY	167	23.701		35.863	1.00		3
ATOM	1221	N	SER	168	24.504		37.909	1.00		-
MOTA MOTA	1222	CA	SER	168	24.434		38.252	1.00		-5
ATOM	1223 1224	CB OG	SER SER	168 168	23.543 22.558		39.465	1.00		3 3
ATOM	1225	C	SER	168	25.820		39.118 38.537	1.00		3
ATOM	1226	ŏ	SER	168	25.961		38.506	1.00		7
MOTA	1227	:1	VAL	169	26.808		28.789	1.00		•
ATOM	1228	CA	VAL	169	28.218		39.149	1.00		• 5
ATOM	1229	CB	VAL	169	28.719		38.657	1.00		ş
ATOM	1230		VAL	169	30.262		38.769	1.00		5
ATOM	1231		VAL	169	28.40		37.197	1.00		
ATOM ATOM	1232	C	VAL	169	28.38		40.666	1.50		-5
ATOM	1233 1234	и И	VAL	169	28.222		41.313	1.00		;
ATOM	1234	CA	GLN GLN	170 170	28.725 28.905		41.201	1.00	15.91	
ATOM	1236	CB	GLN	170	27.92		42.647 43.231	1.00	17.12	÷.
ATOM	1237	SG	GLN	170	27.92		44.766	1.00		7
ATOM	1238	CD	GLN	170	28.20		45.365	1.00		ė.
ATOM	1239	OE1		170	27.36		45.247	1.00		4
MOTA	1240	NE2	GLN	170	29.33	5 33.86%	46.004	1.00		

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ATOM			GLN	170		30.34		6.030			.00 14.		
ATOM	1242		GLN	170		30.73		4.892			.00 10.4	_	
ATOM	1243		ARG	171		31.10 32.47		36.932 36.643			.00 13.		
ATOM	1244		ARG ARG	171 171		33. 4 4		37.71			.00 13.	16 6	
ATOM	1245 1246	CB	ARG	171		33.54		37.81		2.049	.00 12.	_	
ATOM ATOM	1247	CD	ARG	171		34.46		36.75			.00 13.		
ATOM	1248	NE	ARG	171		34.62		36.92			00 10.		
ATOM	1249	CZ	ARG	171		35.27 35.84		37.93 38.89			1.00 4.		
MOTA	1250	NH1 NH2		171 171		35.30		38.00					;
MOTA MOTA	1251 1252	C	ARG	171		32.58		36.54	3 4		1.00 15.		5
ATOM	1253	0	ARG	171		31.70		37.06			1.00 17.		3 7
ATOM	1254	N	VAL	172		33.6		35.91 35.72			1.00 11. 1.00		, 5
ATOM	1255	CA	VAL	172 172		33.83 33.4		34.26			1.00 10.		6
MOTA	1256 1257	CB	VAL VAL	172		33.3		34.15		9.521			5
atom Atom	1258		VAL	172		32.2		33.74		7.262	1.00 11.		<u>.</u>
ATOM	1259	Ç	VAL	172		35.2		35.96		8.031	1.00 9.		6 3
ATOM	1260	0	VAL	172		36.1		35.39		9.062	1.00 14	-	7
MOTA	1261	N	GLU	173 173		35.3 36.6		37.04		9.657	1.00 14		5
ATOM	1262 1263	CA CB	GLU	173		36.7		38.4		0.218	1.00 17		5
atom Atom	1264	CG	GLU	173		36.5		39.5		19.173	1.00 21		5
ATOM	1265	CD	GLU	173		37.2		40.9		19.573	1.00 25		ა ვ
ATOM	1266		GLU	173		37.7		41.6		18.649 50.803	1.00 25		3
ATOM	1267		GLU	173 173		36.9		36.0		50.779	1.00 13		÷
ATOM	1268 1269	C	GLU	173		36.0		35.7	20	51.592	1.00 13		3
atom Atom	1270		ILE	174		38.0		35.4		50.719	1.00 14		7
ATOM	1271	CA	ILE	174		38.		34.4		51.669 50.966	1.00 14		6 6
MOTA	1272		ILE	174		38.5 40.5		33.0		51.689	1.00 12		5
MOTA	1273		2 ILE 1 ILE	174 174		37.		32.1		50.893	1.00 13		6
MOTA MOTA	1274 1275		1 ILE	174		36.		32.6		49.917	1.00 12		6
MOTA	1276		ILE	174		39.		35.0		52.250	1.00-1		6 8
ATOM	1277		ILE				563	35.€		51.532 53.558	1.00 1		7
ATOM	1278		LEU				982 138	34.9		54.166	1.00 1		6
ATOM	1279						838	35.9		55.609	1.00 1		6
ATOM	1280						467	37.4		55.733	1.00 1		6
MOTA MOTA	1282	-	1 LEU				100	38.		54.394	1.00 1		6
ATOM	1283		2 LEU				345	37.		56.733 54.031	1.00 1		ó ó
ATOM	128		LEU				.394 .322	34. 33.		53.838	1.00 1		3
MOTA			LEU GLU				542	35.		54.084	1.00 1		7
MOTA MOTA						44.	. 842			53.946	1.00 1		5
ATOM				J 17			.000		733	54.145	1.00 2		5 5
MOTA	128						.963 .145		472 925	55.432 55.180	1.00 2		6
ATOM							.330		343	55.218	1.00 2		s
ATOM		_	E1 GL				.117		626	54.911	1.00 2		3
ATOM ATOM		-	GL				.068		602	54.852	1.00 1		é
ATOM							.875		686	56.062 54.259		9.95	3 7
ATOM							.574 .839		. 54 5 . 34 1	55.001		8.11	5
ATOM							.738		.340	54.827		7.43	÷
MOTA MOTA							. 990		.169	54.962		9.00	â
ATON				G 1	78		.534		.787	54.493		7.50	7
ATOR	4 130		A AR		78		2.39		.882 .660	54.31		8.26 10.81	5
ATO			B AR		78		L.11 L.15		. 621	55.61		14.76	ś
ATO! ATO!			G AF		78 78		0.91		.920	56.95	i.00	20.12	÷
ATO			IE AF		78		1.90		. 285	57.96		24.00	7
ATO		05 0	Z AF	RG 1	78		2.40		.509	58.13		26.21	÷ 7
ATO	M 13		H1 A		78		2.00		.543	57.38 59.04		27.32 26.51	7
ATO			H2 Al		78 78		3.35 2.37		.216			7.67	
ato ato					78		2.48		.881	51.93	8 1.00	8.54	3
ATO					79	4	2.20	5 27	.906			7.97	7
ATO	M 13	11 '	CA T	HR 1	79		2.14		7.157			9.51 9.72	6
ATO					79		3.37		5.310 5.703			12.75	
ATC			OG1 T CG2 T		.79 .79		4.55		7.162			6.02	
ATC ATC					79		0.8	73 20	6.265	51.64	1 1.00	14.19	
ATO	OM 13	116	0 T	HR 1	179		0.8		5.102			15.46	
ATO					180		9.7		6.831 6.188			13.36	
ATO	rri 13	313	CA G	LU	180	-	8.4	U	J. 100		- 4.00		

bref2	lc.pd	b		Thu	Apr	25 1	.2:2	7:47	1996	18	
MOTA	1319	CB	GLU	180	3	8.329	25	.242	53.340	1.00 14.42	ć
MOTA	1320	CG	GLU	180		7.418		.052	53.048	1.00 18.37	ó
ATOM	1321	CD	GLU	180		7.112		.255	54.299	1.00 19.86	é
ATOM	1322	OE1		180		6.526		.877	55.216	1.00 21.31	}
ATOM	1323	OE2		180		7.473		.045	54.387	1.00 18.58	ò
ATOM	1324	C	GLU	180		7.442 7.742		.288	52.301 52.782	1.00 14.56	5
ATOM ATOM	1325 1326	N O	GLU CYS	180 181		6.209		.385 5.986	51.934	1.00 14.76 1.00 13.82	è 7
ATOM	1327	CA	CYS	181		5.149		9.967	52.034	1.00 13.62	6
ATOM	1328	CB	CYS	181		5.382		990	50.936	1.00 12.66	5
MOTA	1329	SG	CYS	181		3.911		. 643	50.288	1.00 13.38	15
ATOM	1330	C	CYS	181		3.766		.287	51.905	1.00 13.84	-6
ATOM	1331	0	CYS	181	3	3.606	2€	3.383	51.086	1.00 15.56	8
ATOM	1332	N	VAL	182	3	2.790	27	1.639	52.743	1.00 13.12	7
MOTA	1333	CA	VAL	182		1.478		. 985	52.613	1.00 11.97	6
ATOM	1334	CB	VAL	182		1.093		5.072	53.820	1.00 9.54	5
MOTA	1335	CG1		182		2.003		5.307	55.003	1.00 10.81	6
ATOM	1336 1337	C	VAL	182 182		9.669 0.353		5.255 7.910	54.193 52.171	1.00 8.15	5
ATOM ATOM	1338	0	VAL	182		9.930		3.828	52.872	1.00 13.90	6 3
ATOM	1339	N	LEU	183		9.954		7.715	50.930	1.00 11.79	7
ATOM	1340	CA	LEU	183		8.921		3.515	50.338	1.00 12.76	5
ATOM	1341	СВ	LEU	183		9.052		3.500	43.817	1.00 13.26	5
ATOM	1342	CG	LEU	183		0.193		9.380	43.350	1.00 11.81	5
ATOM	1343	CD1	LEU	183	3	0.636	21	3.956	46.970	1.00 8.24	ર્સ
ATOM	1344	CD2	LEU	183	2	9.734	. 3	0.852	45.398	1.00 13.01	き
ATOM	1345	С	LEU	163		7.564		B.027	50. 7 78	1.00 14.24	5
MOTA	1346	0	LEU	183		7.139		6.887	50.514	1.00 15.09	ક
ATOM	1347	N	SER	184		6.897		8.909	51.487	1.00 14.69	7
ATOM	1348	CA	SER	184		5.583		B.642	51.998	1.00 16.60	6
ATOM	1349	CB	SER Ser	184		5.558 6.601		9.046 8.369	53.461	1.00 17.40	6
ATOM ATOM	1350 1351	og c	SER	184 184		4.671		9.537	54.144 51.208	1.00 19.79	ā 6
ATOM	1352	0	SER	184		25.115		0.545	53.679	1.00 18.84	3
ATOM	1353	N	ASN	185		23.422		9.140	51.048	1.00 18.50	7
ATOM	1354	CA	ASN	185		22.479		9.998	50.338	1.00 21.04	6
ATOM	1355	CB	ASN	185		22.463		1.389	51.008	1.00 27.82	6
ATOM	1356	CG	ASN	185	2	22.274	3	1.330	52.546	1.00 33.52	6
ATOM	1357		ASN	185		22.899		2.131	53.270	1.00 36.61	3
ATOM	1358		ASN	185		21.392		0.414	53.050	1.00 36.25	7
ATOM	1359	C	ASN	185		22.641		0.149	49.794	1.00 19.48	6
ATOM	1360	0	ASN	185		22.967		1.228	43.263	1.00 19.46	ê 7
ATOM	1361 1362	N CA	LEU LEU	186 186		22.329 22.384		9.062 8.972	43.093 46. 63 5	1.00 17.53	έ
ATOM ATOM	1363	CB	LEU	186		23.632		8.170	46.201	1.00 14.99	6
ATOM	1364	CG	LEU	136		25.006		8.318	45.924	1.00 15.24	5
ATOM	1365		LEU	186		25.951		7.172	45.540	1.00 13.51	5
ATOM	1366		LEU	136		25.689		9.663	46.637	1.00 14.02	5
ATOM	1367	ε	LEU	136		21.06		8.230	45.261	1.00 16.15	6
ATOM	1368	0	LEU	186		20.44	9 2	7.566	47.116	1.00 16.68	a
MOTA	1369	N	ARG	187		20.61		8.382	45.019	1.00 15.66	7
MOTA	1370	CA	ARG	187		19.37		7.749	44.576	1.00 14.27	5
MOTA	1371	CB	ARG	187		18.84		8.415			é
ATOM	1372	CG	ARG	187		19.15		9.870	43.263	1.00 19.73	5
ATOM	1373	CD	ARG	187 187		18.52 19.21		30.512 30.197	42. 054 40. 9 05	1.00 23.74	5 7
ATOM ATOM	1374 1375	NE CZ	ARG ARG	187		18.99		29.109	40.060	1.00 26.90	, ÷
ATOM	1376			187		18.11		28.181	40.430	1.00 29.72	i
ATOM	1377		ARG	187		19.59		29.001	33.874	1.00 21.36	
ATOM	1378	C	ARG	187		19.52		26.264	44.298	1.00 16.07	
MOTA	1379	0	ARG	137		20.60	8 3	25.788	43.872	1.00 14.20	3
MOTA	1380	N	GLY	138		18.41		25.557	44.483	1.00 15.94	
MOTA	1381	CA	GLY	188		18.36		24.124	44.291	1.00 17.35	ē
MOTA	1382	C	GLY	188		19.30		23.695	42.842	1.00 19.74	
ATOM	1383	2	GLY	188		17.76		24.421	42.016	1.00 20.69	
MOTA	1384	N	ARG	139		18.82		22.492	42.563	1.00 20.12	
ATOM ATOM	1385 1386	CA	ARG ARG	139 139		18.89		21.885 21.501	41.239	1.00 20.15	
ATOM	1385	CG	ARG	189		17.45		20.203	23.871	1.00 25.04	
ATOM	1388	CD	ARG	139		17.78		20.447	33.380	1.00 25.92	
ATOM	1389	NE	ARG	189		18.57		19.373	37.756	1.00 27.40	
ATOM	1390	CZ	ARG	189		18.07		18.215			
ATOM	1391		1 ARG	169		16.76	36	17.937	37.405	1.00 30.45	;
MOTA	1392		2 ARG	189		18.86		17.342			
ATOM	1393	Ç	ARG	189		19.61		22.773			
ATOM	1394	၁	ARG	199		19.40		22.605			
MOTA MOTA	1395 1396	N CA	THR	130 190		20.43		23.719 24.611			
0.,	2000	- CA	• ***							1.00 17.0	- 7

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ATOM	1397 CB	THR	190	21.494	25.944	40.460	1.00 15.30 5
MOTA	1398 OG1		190	20.370	26.366	41.226	1.00 18.33 E
MOTA	1399 CG2		190	21.869	26.984 24.017	39.390 39.612	1.00 17.97
MOTA	1400 C	THR	190 190	22.576 23.024	23.222	40.428	1.00 17.12
MOTA	1401 0 1402 N	THR ARG	191	23.262	24.460	38.563	1.00 18.62
MOTA MOTA	1402 N	ARG	191	24.621	24.018	38.253	1.00 18.64 5 1.00 23.05 5
ATOM	1404 CB	ARG	191	24.783	23.686	35.746 35.27B	1.00 23.05 5 1.00 28.15 5
MOTA	1405 CG	ARG	191	26.243 26.802	23.477 22.032	35.502	1.00 29.37
ATOM	1406 CD 1407 NE	ARG ARG	191 191	26.824	21.206	25.274	1.00 31.41
ATOM ATOM	1407 NE 1408 CZ	ARG	191	27.677	21.329	34.236	1.00 30.79
ATOM		ARG	191	28.650	22.261	34.198	1.00 30.54 7
ATOM	1410 NH2	ARG	191	27.562	20.481	33.210 38.627	1.00 30.20 7 1.00 15.56 5
MOTA	1411 C	ARG	191	25.471 25.174	25.213 26.344	38.233	1.00 14.09 3
MOTA	1412 ° 1413 N	ARG TYR	191 192	26.495	24.950	39.417	1.00 12.55 7
ATOM ATOM	1413 N 1414 CA	TYR	192	27.380	25.971	39.901	1.00 11.03 5
ATOM	1415 CB	TYP	192	27.283	26.027	41.411	1.00 10.18 6 1.00 13.18 6
ATOM	1416 CG	TYR	192	26.063	26.759 28.138	41.890 42.101	1.00 14.17 6
ATOM	_	LTYR	192 192	26.105 24.949		42.435	1.00 14.60 5
MOTA	1418 CE:	TYR TYR	192	24.837		42.039	1.00 14.10 5
ATOM ATOM		2 TYR	192	23.670		42.371	1.00 15.93
ATOM	1421 CZ	TYR	192	23.745			1.00 13.34
ATOM	1422 OH	TYP.	192	22.618			1.00 12.33
ATOM	1423 C	TYP	192 192	28.759 29.134			1.00 13.81 8
ATOM	1424 0 1425 N	TYP. THR	193	29.51			1.00 10.45
ATOM ATOM	1426 CA		193	30.87			1.00 7.07 f 1.00 7.66 f
ATOM	1427 CP		193	31.03			
MOTA		1 THR	193	30.030 32.39			
MOTA		2 THR THP	193 193	31.68			1.00 7.05 5
MOTA MOTA	1430 C 1431 O	THR	193	31.37	_		
MOTA	1432 N	PHE	194	32.68			
ATOM	1433 C		194	33.48			
MOTA	1434 C		194	33.42 32.03			
ATOM	1435 C	D1 PHE	194 194	31.53			3 1.00 5.87 é
ATOM ATOM		D2 PHE	194	31.22		5 43.51	
ATOM		E1 PHE	194	30.27			
ATOM		E2 PHE	194	29.95 29.48			
MOTA			194 194	34.92			4 1.00 5.55 5
ATOM ATOM				35.3		4 39.93	
ATOM			195	35.64			
ATOM		A ALA		37.05 37.1			
ATOM		B ALA		37.7			
ATOM ATOM				37.1			1 1.00 2.79
HOTA	7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7			39.0		39 41.77	
ATON	1 1449	A VAI		39.8			
OTA		B VAI		40.5 40.2			
ATON ATON		CG1 VAI		40.1			9 1.00 4.04 6
ATO		C VA		41.0			95 1.00 2.07 6
ATO			L 196	41.4			
OTA		N AR		41.5 42.6			
ATO		ca ari Cb ar		42.4			69 1.00 2.00 5
ATO ATO		AA DO		41.3		10 41.5	74 1.00 2.00 5
ATO		CD AR	G 197	41.0			
ATO		NE AR		40.			
OTA		CZ AR NH1 AR		40.			57 1.00 2.00 7
ATC ATC		NH2 AP					93 1.00 4.02
ATC		C AP		43.	374 33.		
ATC	M 1465	O AF					
ATO		N AI		_	710 33. 475 33.		199 1.00 2.00
TA Ta		CA AI			420 32.		
ATC		C Al		46.	241 35.	326 44.	
AT		O A	LA 198	46.	614 35.		
TA			RG 199	_		901 45. 171 45.	
TA TA			RG 199 RG 199			304 45.	
	OM 1473		RG 19			669 45.	

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ATOM	1475	CD	ARG	199	45.9	38	40.737	45.915	1.00	9.17	5
MOTA	1476	NE	ARG	199	46.3	06	42.120	45.579	1.00		-
MOTA	1477	CZ	ARG	199	46.1		42.662	44.363	1.00	15.94	٤
ATOM	1478	NH1		199	45.7		41.950	43.339	1.00		7
ATOM	1479	NH2		199	46.4		43.954	44.181		18.45	7
ATOM	1480	C	ARG ARG	199 1 99	48.0 47.5		37.321 36.916	47.023	1.00	5.53	5
ATOM ATOM	1481 1482	N O	MET	200	49.2		37.864	48.058 46.984	1.00	8.08	-
ATOM	1483	ÇA	MET	200	50.0		38.096	48.197	1.00	5.53 4.85	5
ATOM	1484	CB	MET	200	51.4		38.423	47.891	1.00	3.73	5
ATOM	1485	CG	MET	200	52.3	11	37.271	47.346	1.00	4.67	5
MOTA	1486	SD	MET	200	53.2		36.286	48.538	1.00	9.73	16
MOTA	1487	CE	MET	200	52.2		34.975	48.812	1.00	2.41	5
MOTA	1488 1489	C	MET	200	49.3		39.289	48.874	1.00	7.02	5
ATOM ATOM	1499	N O	MET ALA	200 201	49.0 49.0		40.314 39.126	48.228 50.167	1.00	6.42	3 -
ATOM	1491	CA	ALA	201	48.3		40.140	50.962	1.00	7.96 10.65	5
ATOM	1492	СВ	ALA	201	47.6		39.474	52.117	1.00	4.85	6
ATOM	1493	С	ALA	201	49.2	61	41.285	51.464		12.36	5
ATOM	1494	0	ALA	201	50.4	188	41.204	51.453		13.02	3
ATOM	1495	N	GLU	202	48.6		42.360	51.901	1.00	15.72	7
ATOM	1496	CA	GLU	202	49.3		43.527	52.421	1.00	19.04	5
ATOM	1497	CB	GLU	202	48.4		44.756	52.276		23.13	5
ATOM	1498	CG	GLU	202	47.6		44.796	50.914		28.94	5
ATOM ATOM	1499 1500	CD	GLU GLU	202 202	48.3 49.4		45.575	49.757		31.22	÷ .
ATOM	1501	OE2	GLU	202	47.7		46.164 45.613	49.968 48.634		32.80 30.41	3
ATOM	1502	ç.	GLU	202	49.7		43.317	53.903		19.11	•
ATOM	1503	0	GLU	202	49.3		42.327	54.561		20.41	3
ATOM	1504	N	PRO	203	50.6	596	44.173	54.411		16.25	7
ATOM	1505	CD	PRO	203	51.1		44.143	55.820	1.00	15.32	5
ATOM	1506	CA	PRO	203	51.3		45.290	53.714		14.26	5
MOTA	1507	CB	PRO	203	51.3		46.367	54.782		13.02	6
ATOM ATOM	1508 1509	CG	PRO PRO	203 203	51.8 52.7		45.538	55.984		16.38	5
ATOM	1510	0	PRO	203	53.5		44.892 45.743	53.356 52.985		12.03 15.28	6 3
ATOM	1511	N	SER	204	53.0		43.623	53.540	1.00	8.98	7
ATOM	1512	CA	SER	204	54.4		43.146	53.222		11.79	5
ATOM	1513	CB	SEP.	204	54.6	674	41.764	53.868		11.87	5
MOTA	1514	OG	SER	204	55.0	93	41.356	55.224		12.48	=
MOTA	1515	С	SER	204	54.6		43.060	51.696		11.88	5
MOTA	1516	0	SER	204	55.6		43.660	51.152		11.24	5
ATOM	1517	N	PHE	205	53.8		42.309	51.031		10.89	7
atom Atom	1518 1519	CA CB	PHE PHE	205 205	53.9 53.9		42.074 40.573	49.624 49.390	1.00	8.76	ź
ATOM	1520	CG	PHE	205	55.0		39.862	50.052	1.00	8.70 12.81	5 6
ATOM	1521		PHE	205	54.1		38.885	51.029		11.19	÷
ATOM	1522		PHE	205	56.3		40.136	49.668		11.00	ě.
MOTA	1523	CE1	PHE	235	55.9	921	38.198	51.599	1.00	7.35	÷
MOTA	1524	CE2	PHE	205	57.4		39.449	50.237	1.00	11.11	£
MOTA	1525	CZ	PHE	205	57.		38.480	51.202	1.00	8.98	ē
ATOM	1526	C	PHE	205	52.		42.728	48.900	1.00	8.87	÷
ATOM ATOM	1527 1528	O N	PHE GLY	205 206	51. 52.	756 913	43.147 42.864	49.508 47.592	1.00		=
ATOM	1529	CA	GLY	206	51.		43.459	46.751	1.00	8.57 8.14	7. 6
ATOM	1530	c	GLY	206	52.		42.855	45.367	1.00	7.24	Ę
ATOM	1531	0	GLY	206	52.		42.124	45.081	1.00	8.58	
MOTA	1532	. N	GLY	207	51.		43.080	44.520	1.00	7.18	5
MOTA	1533	CA	GLY	207	51.		42.534	43.176	1.00	7.59	÷
MOTA	1534	С	SLY	2.07	49.		42.355	42.430	1.00	4.80	÷
ATOM	1535	٥	GLY	207	48.		43.048	42.656	1.00	5.05	= = = = = = = = = = = = = = = = = = = =
ATOM	1536	N	PHE	208	49.		41.332	41.608	1.00	3.71	
ATOM ATOM	1537 1536	CA	PHE	208 208	48. 49.		41.069	40.805	1.00	3.73	÷
ATOM	1539	CG	PHE	238		158	42.013	39.322 39.011	1.00	6.46 6.53	•
ATOM	1540		PHE	208		956	43.377	39.004	1.00	6.75	÷
ATOM	1541		PHE	208		441	41.530	28.793	1.00	9.68	5
ATOM	1542		PHE	238		022	44.253	38.790	1.00	7.99	-
ATOM	1543		PHE	208		506	42.393	38.579	1.00	8.12	÷
MOTA	1544	CZ	PHE	208		292	43.756	38.580	1.00	6.95	•
ATOM	1545	Č	PHE	208		896	39.767	41.149	1.00	2.2:	5
ATOM ATOM	1546 1547	;;	PHE TP.P	208		463 603	38.823 39.780	41.704	1.00	2.77	3
ATOM	1548	CA	TP.P	209 209		766	38.625	40.878 41.073	1.00	2.30	;
ATOM	1549	CB	TRP	209		302	38.979	40.811	1.00		:
MOTA	1550	CG	TRP	209		505	39.378	42.011	1.00		
MOTA	1551		2 TPP	209		15€	38.550	43.104	1.00		5 3
ATOM	1552	CE:	2 TP.P	209	42.	347	39.316	43.959	1.00	2.87	;

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ATOM	1553	CE3	TRP	209	4	13.44	15		234	43.446	1.00		ŧ.
ATOM	1554	CD1		209		12.90			586	42.240	1.00		8 7
ATOM	1555	NE1	TRP	209		12.2			554	43.396	1.00		E
MOTA	1556	CZ2		209		41.8			.309 .729	45.148	1.00	4.57	5
ATOM	1557		TRF	209		42.9 42.1			.513	45.461	1.00	4.76	ā.
MOTA	1558		TRP	209 209		46.2			604	40.033	1.00	3.17	÷
ATOM	1559	0	TRP TRP	205		46.5			. 969	33.920	1.00	3.26	3
ATOM	1560 1561	N	SER	210		46.2		36	.335	40.412	1.00	4.99	:
ATOM ATOM	1562	CA	SER	210		46.6	50		.269	39.533	1.00	5.26	ć
ATOM	1563	CB	SER	210		46.9			.002	40.337	1.00	4.60 3.40	<u>ئ</u> ق
ATOM	1564	OG	SER	210		45.6			.363	40.660	1.00	9.36	6
ATOM	1565	C	SER	210		45.5			.968 .689	38.318		13.86	÷
ATOM	1566	0	SER Ala	210 211		45.8			. 924	37.735		10.41	7
ATOM ATOM	1567 1568	N CA	ALA	211		44.8		33	.423	36.757		10.30	ē.
ATOM	1569	СВ	ALA	211		45.€			.571	35.768		10.37	5 5
ATOM	1570	С	ALA	211		43.8			.558	37.567 38.706		11.25 14.78	ŝ
MOTA	1571	0	ALA	211		44.1			.175	37.014	1.00	9.47	,
MOTA	1572	N	TRP	212 212		41.			. 433	37.734	1.00	7.74	5
ATOM	1573 1574	CA CB	TRP TRP	212		40.			.434	36.993	1.00	9.05	5
ATOM	1575	CG	TPP	212		39.			2.765	36.942	1.00	4.98	6
ATOM ATOM	1576		2 TRP	212		39.	061		3.399	33.030		2.00	÷
ATOM	1577		2 TRP	212		38.			4.597	37.547		2.33	é é
ATOM	1578		3 TRP	212		38.			3.063	19.367		2.00 2.00	5
ATOM	1579		1 TRP	212			566		3.576 4.68 0	35.867 36.219		2.00	-
MOTA	1580		1 TRP	212 212			850 811		5.470	38.359			ક
MOTA	1581		2 TRP 3 TRP	212			162		3.921	40.167			ક
ATOM ATOM	1582 1583		2 TRP	212			640		5.111	39.671			6
MOTA	1584		TRP	212		42.	340		0.012				5
ATOM	1585		TRP	212			262	_	9.696			9.63	3
ATOM	1586		SEF	213			771		9.145 7.747			11.60	5
ATOM	1587			213			. 222 . 041		7.183			12.78	ě
MOTA	1586			213 213			667		7.131			13.18	ទ
ATOM	1589 1590		S SER SER	213			.303		6.959			12.67	5
ATOM ATOM	159		SER	213			. 265	5 2	27.471			14.82	3
MOTA	159		GLU	214	l		. 644		25.718			12.59	
MOTA	159			214			.694		24.971 23.661			0 16.37	ક
ATOM	159			214			.307		23.79			0 23.12	á
ATOM	159 159			214 214			.249		24.29			0 27.82	÷
ATOM ATOM	159		E1 GLU	214			. 62		25.33			0 29.07	â
ATOM	159		E2 GLU	21	4		.21		23.63			0 27.91	3
MOTA	159						.55		24.81			0 11.57	€ ±
ATOM	160						.79		24.62 25.03			0 11.02	-
ATOM	160						3.30		25.36			0 12.93	÷.
ATOM	160	_	D PRO				1.06		24.96			0 11.49	5
MOTA MOTA	160 160		B PRO				5.15		25.89		90 1.0	0 9.49	5
MOTA			G PRO				6.43		25.44			00 12.12	5 5
ATOM			PRO				5.37		23.60			00 9.78 00 12.44	
ATOM			PRO				6.66 5.44		22.55				ŧ
ATOM			n vai Ca vai				4.66		22.34				
ATOM MOTA							4.74		21.82				÷
ATOM			CG1 VA	21			5.5		20.5		16 1.	00 9.46	
MOTA			CG2 VA		16		5.22		22.9			00 6.68 30 9.31	
ATON			C VA		16		3.20		24.0		45 1.	00 10.20	
ATC			O VAI		16 17		2.3		21.9				
ATC			n se Ca se		17		0.9		22.2		166 1.	00 9.51	
ATC:			CB SE		17		0.5		22.1	57 37.3		00 10.53	
ATC			OG SE		17	2	9.6	1 C	23.1			00 13.23	
ATC:		19	C SE		17		0.1		21.2			00 10.93	
STA			O SE		17		0.4		20.0		224	00 10.8	
ATC:		21	N LE		18		29.0 28.2		21.7		102	00 11.1	0 1
ATO		22	CA LE		18 18		28.6		21.2			00 9.6	
OTA Ota		523 524	CB LE		18		27.9		20.5		769 1.	. oc 6.9	
ATC		525	CD1 LE		18		28.2		19.1	.50 43.		.50 9.3	
ATC		626	CD2 LE	TU 2	18		28.€		21.3			.00 8.7	
ATC	M 1	627	C LE		18		26.7		21.3		903	.00 11.9 .00 12.2	÷
ATC		628			218		26.1 25.9		22 20.			.00 12.2	
ATO		629 630			219 219		25.5 24.4		20.			.00 13.9	
OTA	<i>n</i> -1	630	CA L	•				•					

bref2	ref21c.pdb			Thu	Apr :	25 12	2:27:4	7 1996		22	
ATOM	1631	CB	LEU	219	23	.867	18.372	40.209	1.00	13.95	é
ATOM	1632	CG	LEU	219	23	.819	18.429	23.736	1.00	16.57	-5
ATOM	1633	CD1	LEU	219		.857	19.303	37.947		18.05	145
MOTA	1634	CD2	LEU	219		.208	18.410	33.096		15.67	5
ATOM ATOM	1635 1636	0	LEU LEU	219		.080 .378	20.226	42.248		12.96	÷
ATOM	1637	N	THP.	219 220		.501	19.295	42.986		12.64	÷ 7
ATOM	1638	CA.	THP	220		.057	21.472	42.692 44.068		12.52	, ÷
ATOM	1639	CB	THP.	220		.289	22.744	44.250		10.53	5
ATOM	1640	OG1	THE	220		.030	23.330	42.967		14.44	;
MOTA	1641	CG2	THP	220	23	.076	23.704	45.099		13.55	:
ATOM	1642	С	THR	220		.111	20.325	44.368	1.00	11.61	÷
ATOM	1643	0	THP	220		.196	20.053	43.582		13.03	3
ATOM	1644	N	THE	303		.975	42.384	64.372		11.41	7
ATOM ATOM	1645 1646	CA CB	THP.	303 303		.750	41.604	65.597 66.344	1.00	9.49	é
ATOM	1647	OG1	THE	303		.988	43.329	65.963		10.05	ર્ ક
ATOM	164B	CG2	THF.	303		.595	42.033	67.861	1.00	12.80	5
ATOM	1649	С	THR	303		.737	40.103	65.280	1.00	9.93	é
MOTA	1650	0	THR	303	68	.525	39.342	65.838	1.00	9.37	Ē
MOTA	1651	N	TYP.	304		.882	39.690	64.343		10.17	7
ATOM	1652	CA	TYP.	304		756	38.291	6 3.97 3	1.00	9.53	ົວ
ATOM	1653	CB	TYP.	304		.306	37.326	64.148	1.00	7.06	é
ATOM	1654	CG	TYP.	304		.839	37.937	65.585	1.00	7.97	4.
ATOM ATOM	1655 1656	CD1	TYF.	304 304		.003	39.120 39.268	66.072 67.389	1.00	4.80	÷
ATOM	1657	CD2	TYF.	304		.030	36.880	66.486	1.00	3.80 6.93	6 6
ATOM	1658	CE 2	TYF	304		.721	37.015	67.809	1.00	4.43	- 6
MOTA	1659	CZ	TYP	304		.20e	38.211	68.261	1.00	4.88	÷
ATOM	1660	он	TYF	304	63	.886	38.359	69.598	1.00	10.24	3
ATOM	1661	С	TYP	304		.182	38.065	62.554	1.00	8.23	6
ATOM	1662	0	TYP.	304		.277	39.024	61.804	1.00	11.69	5
ATOM	1663	N	SEP	305		1.474	36.819	62.201	1.00	8.34	7
MOTA MOTA	1664 1665	CA CB	SEF.	305 305		.856 .204	36.442	60.843	1.00	9.43	6
ATOM	1666	OG.	SEP.	305		.226	35.705 36.516	60.838 61.427	1.00	13.12	გ 8
ATOM	1667	c	SEP	305		5.736	35.557	60.273	1.00	10.05	6
ATOM	1668	Š	SER	305		.490	34.433	60.754	1.00	10.34	ŝ
ATOM	1669	N	CYS	306		5.093	36.051	59.218	1.00	8.05	7
ATOM	1670	CA	CYS	306		1.968	35.364	58.619	1.00	5.52	5
MOTA	1671	C	CYS	306		1.970	35.039	57.131	1.00	6.70	ē
MOTA	1672	0_	CYS	306		6.609	35.702	56.302	1.00	6.69	3
MOTA	1673	CB	CXS	306		3.738	36.188	58.889	1.00	6.36	- 5
ATOM ATOM	1674 1675	SG N	CYS	306 307		3.703	36.836 34.026	60.556 56.808	1.00	8.87	15
ATOM	1676	CA	HIS	307		1.015	33.504	55.459	1.00	6.09 7.50	7 5
ATOM	1677	CB	HIS	307		S.038	32.519	55.083	1.00	11.44	ě
MOTA	1678	SG	HIS	307	64	1.853	31.183	55.746	1.30	14.32	5
ATOM	1679	CD2	HIS	307	54	1.06€	30.124	55.420	1.00	16.07	÷
ATOM	1680	ND1		307	6.5	5.704	30.723	55.734	1.00	16.54	7
ATOM	1681		HIS	307		5.467	29.448	55. 9 76	1.00	14.82	5
ATOM	1682	NE2	HIS	307		4.478	29.056	56.192		17.24	7
ATOM	1683	5	HIS	307		2.576	33.176		1.00	9.06	5
MOTA MOTA	1684 1685	0 N	HIS PHE	307 308		1.811 2.167	32.990	56.188		11.93	3
ATOM	1686	Ċλ	PHE	308		0.815	33.136 32.725	53.980 53.647	1.00	3.50 6.83	7
ATOM	1687	CB	PHE	308		0.491	33.093	52.167	1.00	7.92	
ATOM	1688		PHE	308		0.530	34.557		1.00		5
MOTA	1689	001	PHE	308		1.140	35.016		1.00	6.64	÷
MOTA	1690		PEE	308		9.935	35.482		1.00	9.42	6 6 5
MOTA	1691		PHE	308		1.152	36.402		1.00		6 4 1
ATOM	1692		PHE	308		9.942	36.870		1.00		-
ATOM ATOM	1693 1694	52	PHE PHE	308 308		0.547 0.689	37.324 31.207		1.35	6.33	:
ATOM	1695	:	PHE	338		1.489	30.434		1.00	5.44	£ .
ATOM	1696	Ň	SLY	309		9.746	30.803		1.00		-
ATOM	1697	SA	SLT	339		9.517	29.331		1.00		
ATOM	1698	C	51.5	309		B.315	23.976		1.50	6.57	4
ATOM	1699	7	SLI	309	5	7.806	29.755	53.316	1.00	8.19	á
ATOM	1700	2,	PF:	310		7.791	27.756		1.00	5.60	3
ATOM	1701	CD	PRI	310		8.486	26.582		1.00	9.04	÷
ATOM ATOM	1702	CA	PRI	310		6.648	27.439		1.00		
ATOM	1703 1704	03 08	PF.I	310 310		6.581 7.958	25.337		1.00		:
ATOM	1705	2	PF.I	310		5.395	25.490 26.000				÷
ATOM	1706	Ī	PEI	310		4.387			00		;
ATOM	1707	2.	LEU	311		5.322			1.00		
MOTA	1708	CA	LET	311		4.145					÷

bref21	lc.pdb)		Thu	Apr	25	12	:27	7:47	1996		23	
ATOM	1709	CB L	.EU	311		53.83	4		437	57.080			-
ATOM				311		52.83	37		277	57.127			£ .
ATOM	_		EU	311		51.52			802	57.619			€ €
MOTA	1712			311		52.68			580	55.781		.32 .95	į.
ATOM			LEU	311		54.34			580 411	56.002 55.540		. 76	
ATOM			LEU	311		53.58			898	56.741		.31	=
MOTA			THP.	312 312		55.68			285	57.075		. 52	£
ATOM			THR THP	312		54.7			732	58.256		.52	ξ.
ATOM	1717 1718	CB :		312		54.8			144	58.476		. 5 6	÷
ATOM ATOM	1719	CG2 1		312		55.1		31.	. 951	59.526		.36	5
ATOM	1720		THR	312		57.1			. 342	57.444		.58	£ .
ATOM	1721		THR	312		57.8			. 352	57.215		.15	:
MOTA	1722		TRP	313		57.6			.477 .653	57.979 58.382		. 32	£
MOTA	1723		TRP	313 313		59.0 59.2			.032	58.992		2.13	
MOTA	1724 1725		TRP TRP	313		58.9			.213	58.158		.28	€.
ATOM ATOM	1725	CD2		313		59.6			.779	57.066	1.00	5.34	5
ATOM	1727	CE2		313		59.0	26	37	.968	56.682		1.38	5
ATOM	1728	CE3	TRP	313		60.8	45		.403	56.382		3.66	1
ATOM	1729	CD1	TRP	313		57.8			.044	58.359		1.69	€ 1
MOTA	1730	NE1		313		57.9			.103	57.488		5.00 4.75	Ŧ.
MOTA	1731		TRP	313		59.4			784	55.656 55.350		4.73 6.62	÷
MOTA	1732		TRP	313		61.3			.222	55.004		5.72	÷
ATOM	1733	CH2		313 313		59.6			2.519	59.389		3.38	ŧ
MOTA	1734 1735	5	TRP	313		58.9			2.186	60.359	1.00	9.40	:
MOTA MOTA	1736	N	VAL	314		60.8			2.216	59.139	1.00	40	
ATOM	1737	C.A.	VAL	314		61.5	533	31	.286	60.013		5.27	•
ATOM	1738	CB	VAL	314		62.			0.110	59.249		4.52	
MOTA	1739		VAL	314		62.1			9.204	60.190		3.24	E E
MOTA	1740		VAL	314		61.			9.333	58.536		3.95 3.62	6
ATOM	1741	С	VAL	314		62. 63.			2.192 2.562	60. 49 9			
ATOM	1742	0	VAL CYS	314 315		62.			2.672	61.724		9.61	3 -
ATOM ATOM	1743 1744	N CA	CYS	315		63.			3.567				-
ATOM	1745	S	CYS	315			417	3	2.948	63.293	1.00 1	0.10	÷
ATOM	1746	č	CYS	315		64.	191	3	1.825				3
ATOM	1747	CB	CYS	315			905		4. B 61				
ATOM	1748	SG	CYS	315			176		5.824			7.84	1 3
MOTA	1749	И	LYS	316			402		3.724			3.33	÷
ATOM	1750	CA	LYS	316			381		3.242 2.320				5
ATOM	1751	CB	LYS	316 316			301		1.444				4
ATOM ATOM	1752 1753	CD	LYS	316			242		0.818			13.72	÷
ATOM	1754	CE	LYS	316			213		1.865			17.21	÷ -
ATOM	1755		LYS	316		71.	029	9 3	2.46			17.34	
ATOM	1756		Γλε	316			141		4.462			11.52	:
MOTA	1757		LYS	316			. 193		5.46			7.91	:
MOTA	1758		PRO	317			. 592		34.51			3.25 7.88	Ē
MOTA	1759		PRC	317 317			.284 .344		33.61° 35.66			10.51	÷
ATOM	1760 1761		PRO PRO	317			. 36		35.41			6.33	5
ATOM ATOM	1762		PRO	317			.38		33.97			5.27	3
ATOM	1763		PRO	317			. 77		35.71			14.13	:
MOTA	1764		PRO	317	•		.53		34.73			14.55	
MOTA	1765		GLN	318			.10		36.B6			16.42	5
MOTA				318			.41		37.13 38.43			16.93	:
ATOM				318 318			.01		38.33		16 1.00	18.24	;
ATOM				318			. 60		39.48		54 1.00	17.19	:
ATOM ATOM			1 GLN	319			.73		39.34		39 1.00	15.50	:
ATOM			2 GLN	318		72	.19		40.64			16.42	
ATOM			GLN			72	2.27	3	37.38	5 66.3		16.28	-
ATOM			GLN		6		. 90		38.23			1:.2-	
ATOM			THR				.25		35.79				-
ATOM	177						9.39		36.05		55 1.00	12.98	
ATOM							3.33		34.93			15.65	
ATOM			I THR				8.91 7.86		34.8			12.39	
ATON			THP THP				8.75		37.4				
1OTA 1OTA			THE				9.14		38.3				
ATON			TYF						37.5		54 1.00	8.68	i
ATO							7.1		39.0				
ATO							5.6		39.1				
ATO							5.3		38.9				
ATO ATO			D1 TYE				5.0. 4.7		37.5				
A10												'	

bref2	lc.pd	lb		Thu	Apr	25	12	:27:47	1996		24	
ATOM	1787	CD2	TYR	404	6	5.29	9	40.071	53.050	1.00	2.00	5
MOTA	1788	CE2	TYF.	404	6	4.99	2	39.918	51.710	1.00	2.00	÷
MOTA	1789	CZ	TYR	404	6	4.70	9	38.650	51.219	1.00	2.53	5
MOTA	1790	ОН	TYP	404	6	4.44	7	38.463	49.891	1.00	6.21	÷
ATOM	1791	C	TYP	404	6	7.37	4	39.373	57.169	1.00	6.87	÷
ATOM	1792	0	TYP.	404		7.45		38.477	58.006	1.00	5.71	÷
MOTA	1793	N	SER	405	6	7.45	3	40.653	57.500	1.00	7.44	7
MOTA	1794	CA	SEP	405		7.58		41.068	58.894	1.00	7.96	÷
ATOM	1795	СВ	SEP	405		8.84		41.887	59.094	1.00	9.81	Ē
ATOM	1796	0G	SER	405		9.98		41.082	59.888	1.00	14.61	9
ATOM	1797	С	SEF.	405		6.33		41.863	53.30 5	1.00	10.09	÷
ATOM	1798	0	SER	405		6.15		43.047	58.975	1.00	10.03	3
ATOM	1799	N	CYS	406		5.46		41.198	60.046	1.00	10.45	7
ATOM	1800	CA	CYS	406		4.22		41.789	60.452	1.00	10.00	ē.
ATOM	1801	C	CYS	406		4.19		42.035	61.938	1.00	10.98	£
ATOM	1802	0	CYS	406		4.90		41.386	62.709		12.25	9
ATOM ATOM	1803 1804	CB SG	CYS	406		3.09		40.827	60.107		12.32	5
ATOM	1805	N	HIS	406 407		3.27		39.951	58.514		12.21	16
ATOM	1806	CA	HIS	407		3.36 3.16		42.987	62.332	1.00	10.98	7
ATOM	1807	СВ	HIS	407		4.00		44.542	63.721	1.00	8.89	5
ATOM	1808	CG	HIS	407		3.77		45.803	64.165		11.52	5
ATOM	1809		HIS	407		4.32		46.233	63.370		12.77	÷
ATOM	1810		HIS	407		2.96		46.832	62.204		11.11	÷
ATOM	1811		HIS	467		3.02		47.837	63.B12		10.97	7
ATOM	1812		HIS	407		3.84		47.499	62.954		10.32	÷
ATOM	1913	C	HIS	407		1.68			61.969	1.00	10.00	
ATOM	1814	ં	HIS	407		1.07		43.614	63.801	1.00	3.26	5
ATOM	1815	N	PHE	408		1.09		43.443	62.789	1.00	10.54	3
ATOM	1816	CA	PHE	408		9.69		43.746	64.976	1.30	7.42	
ATOM	1817	CB	PHE	408		9.28		43.636	65.168	1.00	6.36	5
ATOM	1818	CG	PHE	408		9.44		42.280	66.643 67.218	1.00	5.63	<u> </u>
ATOM	1819		PHE	408		9.67		42.125	68.562		3.30	é
ATOM	1820		PHE	408		9.41		41.158	66.409	1.00	4.11	÷
ATOM	1821		PHE	408		9.88		40.882	69.095	1.00	4.22	5 5
ATOM	1822		PHE	408		9.62		39.885	66.935	1.00	2.80 4.80	ē
ATOM	1823	CZ	PHE	408		9.86		39.751	68.282	1.00	4.71	5
ATOM	1824	C	PHE	408		9.45		45.185	64.736	1.00	6.02	5
ATOM	1825	0	PHE	408		0.37		46.018	64.744	1.00	8.84	3
ATOM	1826	N	GLY	409		8.23		45.463	64.347	1.00	4.91	
ATOM	1827	CA	GLY	409	5	7.86	8	46.791	63.936	1.00	2.33	÷
ATOM	1828	C	GLY	409	5	6.49	4	46.954	64.509	1.00	2.02	÷
MOTA	1829	0	GLY	409	5	5.99	6	46.065	€5.196	1.00	4.33	ş
ATOM	1830	N	PRO	410	5	5.87	ي	48.100	64.299	1.00	2.00	7
MOTA	1831	CD	PRO	410	5	6.49	7	49.286	63.693	1.00	2.98	÷
ATOM	1832	CA	PRC	410	5	4.54	4	48.397	64.788	1.00	3.72	÷
ATOM	1833	CB	PRO	410		4.27		49.754	64.166	1.00	5.67	Ŧ.
ATOM	1834	CG	PRC	410	5	5.62	3	50.390	64.195	1.00	5.29	:
ATOM	1835	Ç	PP.C	410	5	3.52	:5	47.367	64.313	1.00	7.04	÷
MOTA	1836	O	PRO	410	5	2.83	1	46.752	65.137	1.00	3.58	3
ATOM	1837	N	LEU	411	5	3.47	1	47.165	62.987	1.00	6.97	-
ATOM	1838	CA	LEU	411	5	2.54	4	46.233	€2.329	1.00	5.66	ē
ATOM	1839	CB	LEU	411	5	2.25	4	46.674	60.898	1.00	8.28	5
ATOM	1840	CC	LEU	411		1.31		47.803	60.553	1.00	11.17	ŧ
ATOM	1841		LEU	411		0.00		47.519	61.244	1.00	15.07	÷
ATOM	1842		LEU	413		1.88		49.156	60.961		14.05	÷
ATOM	1843	С	LEU	411		3.05		44.831	62.192	1.00	4.04	-5
MOTA	1844		LEU	411		2.36		43.870	62.481	1.00	2.7B	3
ATOM	1845	N	THR	412		4.23		44.705	61.643	1.00	3.16	-
ATOM	1846	CA	THE	412		4.74		43.388	61.431	1.00	2.09	÷
ATOM	1847	CE	THR	412		3.98		42.829	60.244	1.00	2.00	5
ATOM	1848		THR	412		4.15		41.413	60.166	1.00	4.34	•
MOTA	1849		THR	412		4.41		43.523	58.976	1.00	2.00	•
ATOM ATOM	1850	C	THR	412		6.25		43.565	61.220	1.00	2.54	-5
ATOM	1851 1852	C N	THE	412		6.73		44.675	61.376	1.00	3.93	2
ATOM	1852	N CA	TRP	413 413		7.00		42.490	60.964	1.00	3.38	1
ATOM	1854	CA	TRP	413		9.00		42.579	60.747	1.00	4.26	5
ATOM	1855	CC	TRP					41.293	60.115	1.00	3.65	3
ATOM	1856		TRP	413		8.9		40.078	60.909	1.00	2.26	- 5
ATOM	1857		TPP	413 413		9.7		39.734	62.023	1.00	4.36	5
ATOM	1858		TEP	413		59.3° 50.7°		38.418	62.398	1.00	2.99	-5
ATOM	1859		TRP	413		8.1		40.409 39.011	62.745	1.00	5.37	
ATOM	1860		TP.P	413		58.3		37.998	60.667	1.00	2.00	3
ATOM	1861		TPP	413		9.9		37.765	61.546 63.459	1.00	3.14	:
ATOM	1862		TP.P	413		51.3		39.764	63.801	1.00	7.15 7.56	
ATOM	1863		TEP	413		50.9		38.451	64.152	00		
ATOM	1864	C	TF:P	413		58.9		43.720	59.832	1.00		
												-

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ATOM	1865	1	TRF	413	51	B.18	3 7		350	59.115	1.00 7.06
ATOM	1866		VAL	414		0.2			923	59.813	1.00 6.50 7 1.00 6.63 f
ATOM	1867	CA	VAL	414		0.9			921 289	58.957 59.660	1.00 7.88
MOTA	1868	C3	VAL	414 414		1.0° 2.1			072	59.029	1.00 6.76 €
MOTA	1869	CG1 CG2		414		9.7			111	59.547	1.00 3.37 5
MOTA MOTA	1870 1871	032	VAL	414	6	2.2	42	44.	.340	58.533	1.00 9.59 5
MOTA	1872	-	VAL	414		3.1			.296	59.303	1.00 11.73
ATOM	1873	: :	CYS	415		2.2			.820	57.314 56.809	1.00 9.75 7 1.00 9.19 5
MOTA	1874	CA	CYS	415		3.5			.222 .007	55.767	1.00 9.05
MOTA	1875 1876	3	CYS	415 415		3.7			.949	55.189	1.00 8.76
ATOM ATOM	1977	CB	CYS	415		3.2			.882	56.222	1.00 9.11 6
ATOM	1978	\$G	CYS	415		2.0			.071	57.341	1.00 14.13 15 1.00 7.88 7
ATOM	1879	N	LYS	416		55.4			.622	55.581 54.585	1.00 7.88 7 1.00 9.50 6
ATOM	1880	CA	LYS	416		66.3 67.3			.197	55.135	1.00 14.71 5
ATOM	1881	CB	LYS	416 416		6 6 .4			.235	56.144	1.00 19.54 5
ATOM	1882 1883	CD	LYS LYS	416		66.			.629	57.541	1.00 23.24 6
MOTA MOTA	1884	CE	LYS	416		65.1		46	.404	58.599	1.00 23.74 6
ATOM	1885	NZ	LYS	416		66.			.888	59.937	1.00 27.08 7 1.00 12.10 5
ATOM	1886	C	LYS	416		67			2.187	54.27B 55.175	1.00 10.95
MOTA	1887	Ç.,	LYS	416 417		67. 67 .			2.817	52.990	1.00 12.45
ATOM	1888		PRO PRO	417			231		3.561	51.771	1.00 11.38 -
MOTA ATOM	1889 1890		PRO	417			434		1.684	52.671	1.00 11.76
ATOM	1391		PRO	417			394		1.647	51.144	
ATOM	1892	CS	PRO	417			247		3.047	50.780 53.221	
ATOM	1893		PRO	417			845 361		1.868 2.990		1.00 14.95
ATOM	1894		PRO GLN	417 418			400		0.762		1.00 15.69 7
MOTA	1895 1896		GLN	418			753		0.741		1.00 16.01 5
atom Atom	1897			418			933		9.562		
ATOM	1898			418			948		9.963		
ATOM	1899	9 ೮೨		41B			. 580		8.823		
ATOM	190		1 GLN	418			.377		7.668 9.131		
ATOM	190		2 GLN	418			. 478 . 660		10.583		
ATOM	190		GLN GLN	418 418			. 470		9.656		2 1.00 20.26 5
MOTA MOTA	190 190		LYS	510			. 636		15.74		
MOTA	190			510			. 98:		14.82		
ATOM	190			510			.004		15.50		
ATOM	190			510			. 79		44. 72: 44. 78	9 100.09 6 99.98	
ATOM	190			510 510			.14			8 101.30	
ATOM ATOM	190 191			510			.28	1 .	42.90	7 101.71	0 1.30 21.40
ATOM			LYS	510			.03		43.64		2 1.30 21.11 6
ATOM		. 2 0	LYS	510			.11		42.77		
ATOM				511			.08 1.20		43.65 42.50		
ATOM				513 513			2.90		42.83		0 1.00 17.03 6
ATOM ATOM			S PHE	51			. 96		41.64		2 1.00 17.36 5
ATOM			D1 PHE				2.47		40.35		_
ATOM		18 3	D2 PHE				0.59		41.80		
ATOM		19 3	E1 PHE	51			1.63		39.23		
ATON			E2 PHE				9.73 0.2		39.39		
4OTA			Z PHE				5.0		41.62		54 1.00 17.52 🦠
ATON ATON				_			5.4		40.40		13 1.00 15.93
ATO			: GLU				5.4		42.2		JZ
ATO	4 19		CA GLU				6.2		41.5		
ATO			CE GLU				6.5		42.3		75 1.30 28.00
ATO			os Gl u od Sl u				6.8		40.6		01 1.00 30.11 6
ATO			III GL				٦.٤		40.5	07 53.9	
ATO	M 19		E2 GL				5.8		40.0		
ATO	M 13	231	C GL	ت 5 :			37.5		41.1		
ATO			: GL		12		37.9		40.0		
ATO			N SE DA SE		13 13		27.9 39.1		42.0		
ATO ATO		934 935	CF SE		13		39.5		43.3	14 96.	143 1.00 12.70
TA TO		936	IS SE		13		40.3	319	43.0		594 1.00 13.07 3
ATO	M 1	337	: SE	R 5	13		39.		40.8		
ATO	om :	338	: SE		13		4(1.(40.0		
ATO		539 539	E LY		14 14		38.6 37.		40.8		
ATC ATC		940 941	CH FA		14		36.		40.		605 1.30 7.59
TA TA		942	SS LY		14		3			165 100.	
	_										

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ATOM	1943	CD	LYS	514	36.388	41.093 1	101.842	1.00 2.50	Ē
ATOM	1944	CE	LYS	514	36.374	42.393		1.00 2.00	į.
ATOM	1945	NZ	LYS	514	35.665	42.215		1.00 3.28	-
ATOM	1946	С	LYS	514	37.621	38.443	97. 9 59	00 11.50	:
ATOM	1947	0	LYS	514	37.841	37.435	98.620	1.00 13.26	÷
ATOM	1948	13	ALA	515	37.138	38.401	96.716	1.00 10.50	-50
ATOM	1949	CA	ALA	515	36.876	37.117	96.038	1.00 9.26	ŧ
MOTA	1950	CB	ALA	515	36.187	37.366	94.719	1.00 10.33	4
ATOM	1951	C	ALA	515	38.165	36.299	95.806	oo a.a3	- 5
MOTA	1952	0	ALA	515	38.176	35.068	9 5.92 0	1.00 7.Tä	3
ATOM	1953	N	ALA	516	39.241	37.026	95.494	1.00 8.76	7
ATOM	1954	CA	ALA	516	40.562	36.478	95.204	1.00 7.65	÷
ATOM	1955	CB	ALA	516	41.457	37.533	94.614	1.00 €.46	ć
ATOM	1956	c	ALA	516	41.205	35.872	96.419	1.00 7.97	÷
ATOM	1957	0	ALA	516	41.690	34.751	96.353	1.00 8.85	ŧ
ATOM	1958	Ŋ	LEU	517	41.226	36.599	97.530	1.00 8.04	7
ATOM	1959	CA	LEU	517	41.809	36.040	98.743	1.00 5.52	5
ATOM	1960	CB	LEU	517	41.445	36.874	99.947	1.00 3.15	- 6
ATOM	1961	CG	LEU	517	42.141	38.193		1.00 4.53	5
ATOM	1962		LEU	517	41.717	39.177	99.108	1.00 9.66	5
ATOM	1963		LEU	517	41.754	38.683		1.00 4.29	5
ATOM	1964	C	LEU	517	41.271	34.634	98.992	1.00 7.39	8
ATOM	1965	0	LEU	517	42.009	33.751	99.437	1.00 10.93	•
ATOM	1966	N	LEU	518	39.997	34.433	93.648	1.00 3.49	-
ATOM	1967	CA	LEU	518	39.297	33.177	98.857	1.00 7.25	ć
ATOM	1968	CB	LEU	518	37.845	33.467	99.273	1.00 5.35	- 5
MOTA	1969	CG	LEU	518	37.614		160.773	1.00 5.58	÷
ATOM	1970		LEU	518	36.802		100.936	1.00 3.48	ē.
MOTA	1971	CD2	LEU	518	36.951		101.495	1.00 6.87	5
ATOM	1972	Ċ	LEU	518	39.339	32.158	97.733	1.00 9.11	é
ATOM	1973	0	LEU	518	39.185	30.955	97.979	1.00 8.10	3
ATOM	1974	N	ALA	519	39.557	32.623	96.505	1.00 11.23	7
ATOM	1975	CA	ALA	519	39.603	31.726	95.342	1.00 13.55	5
ATOM	1976	CB	ALA	519	39.310	32.481	94.072	1.00 12.74	5
ATOM	1977	C	ALA	519	40.908	30.949	95.209	1.00 15.14	- 6
ATOM	1978	0	ALA	519	41.733	31.215	94.311	1.00 15.55	Ξ
ATOM	1979	N	ALA	520	41.047	29.935	96.068	1.00 17.93	?
ATOM	1980	CA	ALA	520	42.228	29.064	96.115	1.00 19.81	5
ATOM	1981	CB	ALA	520	42.169	28.165	97.371	1.00 20.83	:
ATOM	1982	c	ALA	520	42.579	28.212	94.865	1.00 19.53	ć
ATOM	1983	0	ALA	520	41.764	27.430	94.339	1.00 19.39	3
ATOM	1984	N	ARG	521	43.834	28.352	94.449	1.00 90.00	7
ATOM	1985	CA	ARG	521	44.407	27.633	93.322	1.00 90.00	- 8
ATOM	1986	CB	ARG	521	45.499 45.117	28.484	92.652	1.00 90.00	•
ATOM	1987 1988	CG	ARG	521 521	45.751	29.950	92.441	1.00 90.00	÷
ATOM ATOM	1989	CD NE	ARG	521	45.512	30.871	93.500	1.00 90.00	6
ATOM	1990	CZ	ARG	521	46.279	30.373 29.452	94.854 95.464	1.00 93.00	:
ATOM	1991	NH1		521	47.351	28.95?	94.843		:
	1992			521	45.888			1.00 90.00	
ATOM			ARG			28.889	96.620	1.00 90.00	
ATOM ATOM	1993 1994	0	ARG	521 521	45.018 44.842	26.343 26.022	93.866	1.00 90.00	÷
ATOM	1995	и	ARG	522	45.710		95.032	1.00 90.00	Ē
ATOM	1996	CA	GLY	522	46.338	25.592 24.375	93.022 93.500	1.00 90.00	
ATOM	1997	C	GLY	522	47.851	24.578	93.549	1.00 90.00	6
ATOM	1998	Õ	GLY	522	48.288	25.677	93.891	1.00 90.00	ć
ATOM	1999	N	PRO	523	18.672	23.533	93.225	1.00 90.00	3
ATOM	2000		PRC	523	48.070	22.203	92.929	1.00 90.00	÷
ATOM	2001	CA	PRC	523	50.157	23.469	93.185	1.00 90.00	
ATOM	2002	CB	PRO	523	50.429	22.304	92.201	1.00 90.00	5 6 1
ATOM	20.03	CG	PRO	523	49.277	21.315	92.486	. 00 85.50	
ATOM	2004	S	PRO	523	50.968	24.731	92.741	1.00 90.00 1.00 90.00	
ATOM	2005	Š	PRO	523	50.499	25.517	91.984	1.00 90.00	•
ATOM	2006	N	SLU	524	52.222	24.761	93.180	1.00 24.71	:
ATOM	2007	CA	GLU	524	53.121	25.851	92.829	00 23.63	
ATOM	2009	40	GLU	524	54.289	25.979	93.857	1.00 27.67	1
ATOM	2009	cs	GLU	524	55.487	24.958	93.730	00 23.39	÷
ATOM	2010	CD	GLU	524	55.207	23.507	94.250	1.00 23.39	7
ATOM	2011		GLU	524	54.910	22.603	93.413	1.00 21.33	
ATOM	2012		GLU	524	55.343	23.263	35.484	1.00 29.10	÷
MOTA	2013	c -	GLU	524	53.672	25.532	91.428	1.00 21.32	·
ATOM	2014	Ċ	GLU	524	53.705	24.359	91.016	1.00 21.32	
ATOM	2015	N	GLU	525	54.169	25.564	90.747	1.00 20.22	•
ATOM	2016	CA	GLU	525	54.722	26.411	89.427	1.00 11.50 1.00 13.58	;
ATOM	2017	CB	GLU	525	53.557	26.334	88.442	1.00 15.50	,
ATOM	2018	CG	GLU	525	53.857	25.543	57.149	1.00 27.12	\$
ATOM	2019	CD	GLU	525	52.595	25.163	86.357	1.00 31.94	3
ATOM	2020	OE:	I GLU	525	52.474	23.956	85.991	1.00 33.25	ì

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ATOM	2021	OE2	GLU	525		51.731	26.066			1.00 34		
MOTA	2022		SLU	525		55.572	27.633					
ATOM	2023		GLU	525		55.306	28.676				.70 · 5	
ATOM	2024		LEU	526		56.619	27.495		.331		.14	
MOTA	2025	CA	LEU	526		57.455	28.636	_	.940			:
ATOM	2026	CB	LEU	526		58.859	28.182		.485			
ATOM	2027	CG	LEU	526		60.103	29.08	-	.590			
ATOM	2028	CD1	LEU	526		61.166	28.50		.706 .193			:
ATOM	2029	CD2	LEU	526		59.856	30.49		. 751			ŧ
ATOM	2030	C	LEU	526		56.688	29.24		5.733			:
ATOM	2031	0	LEU	526		56.527			5.892		.00	_
MOTA	2032	N	LEU	527		56.209	30.47		5.854		.00	Ę
ATOM	2033	CA	LEU	527		55.415	31.63		5.441		1.05	ŧ.
MOTA	2034	CB	LEU	527		54.115 53.035	30.65		5.824		2.65	.
ATOM	2035	CG	LEU	527		51.951	31.42		7.441		2.00	•
ATOM	2036		LEU	527		52.547	29.88		5.620		2.00	ŧ
ATOM	2037		LEU	527 527		56.110	32.25		5.176		4.04	€
ATOM	2038	C	LEU	527		56.413	33.25		5.836	1.00	5.30	:
ATOM	2039	0	LEU CYS	528		56.234	32.17		3.844	1.00	3.62	
MOTA	2040	N CA	CYS	528		56.929	33.19		3.051		2.97	ξ.
MOTA	2041	C	CYS	528		55.987	33.81	10 8	2.044		2.18	•
ATOM	2042	0	CYS	528		55.087	33.12	27 8	1.560		2.61	7
ATOM	2043	СВ	CYS	528		58.132	32.5	93 6	2.282		2.00	-
MOTA	2044	SG	CYS	528		59.491	31.8	32 8	3.234		2.00	
MOTA	2045	N N	PHE	529		56.197	35.0	88 E	1.743	00.:	2.00	
MOTA	2046	CA	PHE	529		55.397	35.7	92 8	0.758	1.00	4.16	€.
MOTA	2047	CB	PHE	529		54.008	36.1	43 8	1.303	1.00	3.68	5
ATOM	2048		PHE	529		53.980		15 8	22.231	1.00	2.00	€.
ATOM	2049		PHE	529		53.958		11 8	31.733	1.00	2.00	÷
MOTA	2050		PHE	529		53.912			3.611	1.00	2.00	÷
ATOM	2051		PHE	529		53.868		97 8	32.590	1.00	2.00	÷
ATOM	2052 2053		PHE	529		53.822		07 1	84.471	1.00	2.00	=
MOTA	2054		PHE	529		53.801		90 1	E3.961	1.00	2.00	•
ATOM	2055		PHE	529		56.100	37.0	31	80.200	1.00	5.77	=
ATOM	2056		PHE	529		57.078			80.785		6.52	:
ATOM	205		THR	530		55.663	37.4	171	79.018		2.84	
MOTA	205		THP	530		56.22		555	78.377	1.00	2.00	÷
ATOM	205			530		57.22			77.232		2.00	÷.
MOTA	206		1 THE	530		57.68	3 39.4	460	76.579		2.84	÷
ATOM	206		2 THP	530		56.63	7 37.	355	76.234		2.96	
ATOM	206	_	THP.	530		55.07	6 39.	582	77.948	1.00	2.59	=
ATOM ATOM	206		THR	530		53.99	9 39.	124	77.611		4.31	<u>:</u>
ATOM	206		GLU	531		55.27	5 40.	882	78.076		2.23	
ATOM				531		54.24	6 41.	854	77.747	1.00	5.46	ŧ
ATOM				533		54.17		919	73.836		10.50	
ATOM				533		54.04		346	e0.25	1.55	12.93	:
ATOM		_		533		53.77		413	81.29	3 1.00	14.12	:
ATOM			E1 GLU	5.31		54.08		606	81.07		15.54	•
ATOM			E2 GLU	53	:	53.22		052	£2.35		18.13	
ATOM			GLU	53	<u>:</u>	54.46		489	76.38		6.42	:
ATOM			GLU	53	1	53.50		685	75.65		9.10	;
ATOM			ARG	53	2	55.6	59 43.	.021	76.15		5.91 6.83	Ŧ
ATON			ARC			56.0		.529	74.83		6.46	Ŧ
ATON		75 C				56.9		.795	74.89			
OTA		76 C	G ARC			56.1		.059	75.09			- 2
ATO	4 20					55.6		.070	76.46 76.69	5	14.70	-
ATO	4 20					54.5		. 930	77.89		17.72	- 1
ATO	4 20					54.1		.395	73.97		13.74	:
ATO	9 20		H1 ARC			54.8		.096	73.01		18.08	-
OTA		•	H2 AR			52.9		.056	74.43		9.68	:
ATO	M 20					56.9		.364	75.05	23 . 00	12.29	-
ATO:	M 20	8 3 0				56.9			73.43		10.64	-
ATO					3.3	57.7		.502	73.19		12.12	
ATO	M 20	85 0	IA LE		33	58.6		.356	71.8	21 . 00	13.13	:
ATO			B LE		23	58.3		.790	71.7	41 00	10.95	
ATO			CG LE		33	56.8		298	70.3		11.69	
ATC			D1 LE		33	56.5		2.773	72.7		12.40	
ATC	M 20		CD2 LE		23	56.		204	73.4	30 - 20	0 11.89	
ATC			C LE		23	60.0		.733 . 490		35 L.S.	0 12.70	; :
ATC			O LE		33	60.		1. 59 0 2.115			C 12.95	
TA			N GL		34	60		2.523			13.30	
ATO			CA GI		34	61.		2.323 3.882			C 16.94	
ATO			CB G1		34	61.		4.974	_	91	0 23.08	3
ATO			CG GI		34	51.		6.010			26.0	
ATO			CD GI		34			€.B60			25.3	
AT			OE1 S		34			5.938			25.8	
AT	UM 2	098	OE2 G	-	34	01.	4					

bref2	lc.pc	£Ъ		Thu	Apr 2	5 1:	2:27:4	7 1996		28	
ATOM	2099	С	GLU	534	61.	892	42.579	75.527	1.00	10.95	÷
ATOM	2100	C	GLU	534	62.	651	42.380	77.066		10.92	
ATOM	2101	N	ASP	535	61.	251	41.637	77.194	1.00	9.01	7
ATOM	2102	CA	ASP	535	61.		41.578	78.638	1.00	6.92	₹.
ATOM	2103	CB	ASP	535	60.		42.544	79.128	1.00	8.31	÷
ATOM	2104	CG	ASP	535	58.		42.334	78.430	1.00	8.75	Ę
ATOM ATOM	2105 2106		ASP	535	58.		41.541	78.913	1.00	11.89	3
ATOM	2100	C	ASP ASP	535° 535	58. 60.		42.949	77.372	1.00	15.77	5
ATOM	2108	٥	ASP	535	60.		40.201 39.577	79.033 73.295	1.00	6.27	5
ATOM	2109	N	LEU	536	61.		39.731	80.204	1.00	6.65 5.28	3 7
ATOM	2110	CA	LEU	536	60.		38.436	80.651	1.00	4.48	é
ATOM	2111	CB	LEU	536	61.		37.315	80.149	1.00	2.00	÷
ATOM	2112	CG	LEU	536	61.		35.958	80.495	1.00	2.00	5
MOTA	2113		LEU	536	59.	697	35.789	79.782	1.00	2.00	ē.
ATOM	2114		LEU	536	61.		34.853	80.152	1.00	2.00	é
ATOM	2115	Ċ	LEU	536	60.		38.468	82.154	1.00	5.42	é
ATOM	2116	0	LEU	536	61.		38.896	82.751	1.00	5.81	3
ATOM ATOM	2117 2118	N CA	VAL VAL	537 537	59.		38.093	82.767	1.00	6.59	7
ATOM	2119	CB	VAL	537	59.: 58.		38.050 39.006	84.219	1.00	4,71	5
ATOM	2120	CG1	VAL	537	58.		38.900	84.761 86.262	1.00	3.90	5
MOTA	2121		VAL	537	58.		40.434	E4.386	1.00	7.66 6.66	5
ATOM	2122	C	VAL	537	59.		36.652	E4.604	1.00	2.70	é
ATOM	2123	0	VAL	537	58.		36.096	83.977	1.00	5.62	
ATOM	2124	N	CYS	538	59.	812	36.048	85.553	1.00	3.31	3 7
ATOM	2125	CA	CYS	538	59.		34.711	65.055	1.00	4.73	
ATOM	2126	C	CYS	538	59.		34.771	27.597	1.30	5.86	5
ATOM	2127	೦	CYS	53B	60.		35.457	63.257	1.00	6.30	Ξ
ATOM ATOM	2128 2129	CB SG	CYS	538	60.		33.619	£5.600	1.50	2.00	- 6
ATOM	2130	N	PHE	538 539	60. 58.		33.421	83.795	1.00	3.79	15
ATOM	2131	CA	PHE	539	58.		34.059 34.099	88.178 89.621	1.00	3.78 4.15	7
ATOM	2132	CB	PHE	539	57.		35.232	89.997	1.00	4.13	5 5
MOTA	2133	CG	PHE	539	55.		35.009	89.515	1.00	7.86	5
ATOM	2134	CD1	PHE	539	54.		34.690	90.420	1.00	5.60	6
ATOM	2135	CD2	PHE	539	55.	519	35.104	88.147	1.00	9.65	6
ATOM	2136	CE1	PHE	539	53.	540	34.470	89.986	1.00	4.81	á
ATOM	2137		PHE	539	54.	201	34.878	87.706	1.00	7.22	-5
ATOM	2138	CZ	PHE	539	53.		34.562	88.630	1.00	5.52	Ģ.
ATOM	2139	C	PHE	539	57.		32.807	90.123	1.00	3.30	÷
ATOM ATOM	2140 2141	O N	PHE	539	57.		31.913	89.352	1.00	5.07	3
ATOM	2141	A)	TP.P TP.P	540 540	57. 56.		32.696 31.575	91.436	1.00	2.62	7
ATOM	2143	CB	TRP	540	57.		30.331	92.102 92.252	1.00	5.41 5.13	ó
ATOM	2144	CG	TRP	540	58.		30.380	93.315	1.00	7.06	ē ē
ATOM	2145	CD2	TRP	540	60.		30.807	93.175	1.00	4.64	- 5
ATOM	2146	CE2	TRP	540	60.	861	30.657	94.430	1.00	5.72	4
ATOM	2147	CE3	TPP	540	61.	800	31.299	92.110	1.00	5.86	5
ATOM	2148	CD1	TRP	540		738	29.995	94.610	1.50	8.29	÷
ATOM	2149	NE 1		540	59.		30.161	95.286	1.00	8.36	7
ATOM	2150		TRP	540		208	30.984	94.657	1.00	8.15	÷
ATOM ATOM	2151 2152		TRP	540 540		336	31.623	92.328	1.00	7.58	5
ATOM	2153	C	TRP	540		927 504	31.465 32.189	93. 59 6 93. 4 17	1.00	8.06	÷
ATOM	2154	ő	TRP	540		774	33.366	93.668	1.00	6.24 7.32	3
ATOM	2155	19	GLU	541		698	31.467	94.186	1.00	8.B1	7
MOTA	2156	. CY	GLU	541		187	31.999	95.452		10.45	÷
ATOM	2157	CB	GLU	541		768	32.565	95.270		11.89	-
MOTA	2158	CG	GLU	541	53.	592	33.523	94.070		14.89	5
ATOM	2,59	CD	GLU	541		202	34.134	93.991		16.24	-5
ATOM	2160		GLU	541		094	35.229	93.415		17.33	- 5
MOTA MOTA	2161		GLU	541		219	33.550	94.516		16.64	ì
ATOM	2162 2163	о О	GLU	541 541		14B	30.925 29.811	96.507		10.03	- 5
ATOM	2164	N	GLU	542		552	31.242	95.232 97.724		10.32	:
ATOM	2165	CA	GLU	542		521	30.222	98.766	- 00	10.71	ş
atom	2166	СВ	GLU	542		871	29.482	98.833	1.00	10.78 10.24	5
ATOM	2167	CG	GLU	542		122	30.359		1.00	14.40	é
ATOM	2168	CD	GLU	542		400	29.571	99.006		15.97	
ATOM	2169		GLU	542		711		100.188	1.00	17.03	3
ATOM	2170		GLU	542		095	29.263	98.026	1.00	17.30	3
atom atom	2171 2172	5	GLU	542		.083		100.128	1.00	9.66	:
ATOM	2173	33	GLU ALA	542 543		741		100.248	1.00	9.88	
ATOM	2174	CA	ALA	543		652		101.135	1.00 1.00		
ATOM	2175	30	ALA	543		466		103.325	1.00	7.10 4.26	5 ÷
ATOM	2176	C	ALA	543		716		103.108	1.00		
											•

bref2	lc.pd	b		Thu	Apr 25	12:2	7:47	1996		29	
ATOM	2177	٥	ALA	543	56.911			02.998	1.00 10	. 83 . 48	
MOTA	2178	N	ALA	544	55.286			103.695	1.00 10		
MOTA	2179	CA	ALA	544	56.199	33	.185	104.325 104.890	1.00 10		
ATOM	2180	CB	ALA	544	55.425		397	105.438	1.00 11		
MOTA	2181	c	ALA	544	56.86° 56.169			106.216	00 1		.
MOTA	2182	0	ALA SER	544 545	58.20			105.456	1.00 13		
ATOM	2183	N CA	SER	545	58.99			166.453	1.00 1		٤
ATOM ATOM	2184 2185	CB	SER	545	59.33	5 30		105.980	1.00 1		ξ.
ATOM	2186	OG	SER	545	€0.29			106.827	1.00 1		=
ATOM	2187	C	SEP.	545	60.24			106.891	1.00 1	4.68	€ -
ATOM	2188	С	SER	545	60.86			106.117	1.00 1		-
MOTA	2189	N	ALA	546	60.55 61.63			103.114	1.00 1		£.
MOTA	2190	CA	ALA ALA	546 546	61.92			119.200	1.00 1		ج
MOTA	2191 2192	CB C	ALA	546	62.92			108.143	1.00 1		€
ATOM ATOM	2193	o	ALA	546	63.65			107.751			ξ -
ATOM	2194	N	GLY	547	63.21			107.965	1.00 1		
ATOM	2195	CA	GLY	547	64.43			107.300		0.46	é
ATOM	2196	С	GLY	547	64.84			106.032		20.80	5
ATOM	2197	C	GLY	547	66.04			105.739			5
MOTA	2198	N	VAL	548	63.86			105.322			Ę
MOTA	2199	CA	VAL	548	64.11 63.11			103.826			ŧ
ATOM	2200	CB	VAL	54B 548	63.13			102.363		13.62	5
ATOM	2201		L VAL	548	63.4			104.756	1.00	11.28	÷
ATOM	2202 2203	0	VAL	54B	63.8	74 3	3.971	102.995	5 1.00		ē.
MOTA MOTA	2204	õ	VAL	548	62.7			102.71		16.13	3
ATOM	2205	N	GLY'	549	64.9			102.54	1 1.00	15.42	-
ATOM	2206	CA	GLY	549	64.8		5.667			12.34	5 5
ATOM	2207		GLY	549	65.4			100.26		11.82	3
ATOM	2208		GLY	549	65.7 65.6		3. 9 91			12.01	-
ATOM	2209		PRO	550 550	65.2		37.459			12.99	5
ATOM	2210			550	66.2		5.639			13.59	÷
MOTA MOTA	2211 2212			550	66.3		36.943			9.83	÷
ATOM	2213			550	66.2	01	38.019			10.09	÷
MOTA	2214		PRO	550	67.€		34.964			13.34	÷
ATOM	2215		PRO	550	67.9		34.06			14.83	3
ATOM	2216	5 N	GLY	551	68.3		35.340			13.58	
ATOM	221			551	69.		34.79			9.01	ا ج
MOTA	2218		GLY	551	69.° 70.0		33.30 32.73			11.57	
MOTA	221		GLY	551 552	6B.		32.65			6.84	÷
ATOM	222		ASN ASN	552			31.21			6.10	5
ATOM ATOM	222							1 100.90		4.08	÷
MOTA	222					797	31.44			6.03	1
ATOM	222		DI ASN	552				2 102.8		7.24	3
ATOM	222	5 N	D2 ASN			991		1 102.63 4 98.5		3.39 7.54	ē
ATOM						287	30.50				•
ATOM						176 157	31.27				7
ATOM						867	30.73				Ē
ATOM ATOM	_		B TYP			432	31.08		79 1.00		ć
ATOM			G TYF			367	30.34		20 1.00	4.46	Æ
ATOM			D1 TYF			491	31.00			3.71	=
ATOM		3 0	E1 TYF		_	.574	30.29				: 5
ATOM	223		D2 TYP			280	28.9				÷
ATOM			E2 TYP			. 355	28.2				:
ATON			Z TYI			.516 .650	28.1				•
ATON			H TYI		·	.791	31.2				÷
1OTA			TY			.432	32.3			0 4.35	=
IOTA IOTA			SE!			.845	30.5		980 1.3	0 5.81	-
OTA			A SE			. 622	31.1	09 32.			:
ATO			CB SE			.999	30.4				:
ATO			og se	F 55		.954	29.1	92 92.		0 11.53	÷
ATO	M 22		C SE			.800	30.7				
OTA			O SE			.289	29.5				
ATO			N PH			.574	31.7				
ATO			CA PH CB PH			.734	32.7				
ATO ATO			CG PH			ac	32.5		3350	5.98	ı
ATC			CD1 PH			.423	32.5	309 ES.	567 1.0	00 3.9€	
ATC			CD2 PF	E 5	55 66	.242	32.		019 1.0		
ATC	M 22	52	CE1 PF			3.541	32.		5070 9630	30 6.29 30 3.92	
ATC		253	CE2 P			379	32.4 32.3		963 1.0 196 1.0		
ATC	M 22	254	CZ PI	1.E 3.	55 64	4.030	J Z				-

bref2	1c.pd	ь		Thu	Apr	25	12	:27:47	1996		30	
ATOM	2255	С	PHE	555	6	8.77	و ر	31.759	٤8.337	1.00	6.86	÷
ATOM	2256	0	PHE	555		9.18		32.858	87.945	1.00	8.43	•
ATOM	2257	N	SER	556	6	9.09	5	30.616	E7.740	1.00	7.22	7
ATOM	2258	CA	SER	556	7	0.01	و	30.503	86.619	1.00	6.83	÷
MOTA	2259	CB	SER	556	7	0.96	9	29.315	86.879	1.00	4.30	á
ATOM	2260	OG	SER	556	7	1.92	23	29.587	87.891	1.00	8.78	3
ATOM	2261	C	SER	556		9.33		30.298	85.257	1.00	5.62	÷
atom	2262	0	SER	556		8.53		29.389	85.117	1.00	8.35	÷
ATOM	2263	N	TYR	557		9.68		31.102	84.255	1.00	3.08	7
ATOM	2264	CA	TYP.	557		9.12		30.943	62.924	1.00	3.30	÷
ATOM	2265	СВ	TYP.	557		8.19		32.089	82.569	1.00	2.00	Ş
ATOM	2266	CG	TYP	557		8.83		33.434	82.422	1.00	2.00	á
ATOM	2267	CD1		557		9.40		33.825	81.218	1.00	2.00	5
ATOM ATOM	2268 2269		TYR TYR	557 557		9.85		35.126	81.023	1.00	2.56	÷
MOTA	2270		TYR	557		8.73 9.18		34.36B 35.667	83.434 83.260	1.00	2.00	5 5
ATOM	2271	cz	TYR	557		9.73		36.047	82.051	1.00	2.00 3.10	6
ATOM	2272	ОН	TYR	557		0.12		37.356	81.865	1.00	3.23	5
ATOM	2273	C	TYR	557		0.19		30.834	81.870	1.00	3.33	é
ATOM	2274	0	TYR	557		11.31		31.196	82.090	1.00	4.25	3
ATOM	2275	N	GLN	558	6	9.83	39	30.360	80.695	1.00	3.52	7
ATOM	2276	CA	GLN	55B	7	70.83	31	30.227	79.648	1.00	3.20	÷
ATOM	2277	CB	GLN	55B	7	71.60	3	28.925	79.828	1.00	3.66	Æ
ATOM	2278	CG	GLN	558		2.50		28.598	78.648	1.00	6.55	÷
MOTA	2279	CD	GLN	558		73.1		27.282	73.788	1.00	5.14	÷
ATOM	2280	OE1		558		12.55		26.320	79.183	1.00	6.68	3
ATOM	2281	NE2	GLN	558		14.4		27.229	78.477	1.00	7.23	7
ATOM	2282	C	GLN	558		70.20		3G.20B	73.279	1.00	3.24	É
ATOM	2283	0	GLN	558 559		59.42		29.309	77.977	1.00	2.96	3.7
ATOM ATOM	2 284 2 28 5	N	LEU LEU			70.5		31.189	77.445	1.00	2.00	
ATOM	2286	CA CB	LEU	559 559		59.94 70.0:		31.139 32.487	76.120 75.399	1.00	2.89	÷
MOTA	2287	CG	LEU	559		58.9		33.527	75.792	1.00	2.00 2.00	÷
ATOM	2288		LEU	559		59.1		34.810	75.005	1.00	2.00	5
ATOM	2289		LEU	559		67.6		32.955	75.564	1.00	2.00	5
ATOM	2290	С	LEU	559		70.7		30.060	75.447	1.00		5
MOTA	2291	0	LEU	559		71.9		29.947	75.728	1.00	4.67	5
MOTA	2292	N	GLU	560	-	70.0	91	29.169	74.718	1.00	6.97	7
ATOM	2293	CA	GLU	560	•	70.7	37	28.064	73. 997	1.00	11.03	ક
ATOM	2294	CB	GLU	560		59.7		27.517	72.938	1.00	14.40	-
ATOM	2295	CG	GLU	560		70.2		26.305	72.163		19.08	á
ATOM	2296	CD	GLU	560		69.7		26.207	70.738		20.20	÷
ATOM	2297	OE1		560		69.7		27.202	69.983		25.39	3
MOTA	2298		GLU	560		69.2		25.130	70.346		21.83	3
atom atom	2 299 2300	0	GLU	560 560		71.9 71.9		28.572	73.310		11.71	á
ATOM	2301	N	ASP	561		73.1		29.491 27.970	72.505		10.88	3
ATOM	2302	CA	ASP	561		74.4		28.346	73.648 73.118		13.20	5
ATOM	2303	CB	ASP	561		74.4		28.398	71.589		11.29	- 6
ATOM	2304	CG	ASP	561		74.4		27.038	70.968		13.29	-
ATOM	2305		ASP	561		74.5		26.039	71.725		14.53	â
ATOM	2306		ASP	561		74.2		26.963	69.729		11.84	ě
MOTA	2307	С	ASP	561		74.9		29.667	73.661		17.27	÷
ATOM	2308	0	ASP	561		75.6	63	30.426	72.931	1.00	21.27	3
ATOM	2309	N	GLU	562		74.7		29.972	74.926	1.00	17.40	7
ATOM	2310	CA	GLU	562		75.2		31.218	75.504		16.45	÷
MOTA	2311	CB	GLU	562		ን4.0		32.235	75.652	1.00	20.22	é
ATOM	2312	, CG	GLU	562		73.2		32.450	74.408	1.00	23.17	ē
MOTA	2313	CD	GLU	562		73.9		33.234	73.289		23.82	÷ 3
ATOM ATOM	2314		GLU	562		74.3		34.407	73.511		22.18	3
ATOM	2315 2316	052	GLU	562		73.9 75.7		32.670	72.169 75.871		27.47	3
MOTA	2317	õ	GLU GLU	562 562		75.4		30.847 29.759	77.373		14.28 15.04	
ATOM	2318	N	PRO	563		76.6		31.581	77.465	1.00	11.29	
ATOM	2319	CD.	PRI	563		77.2		23.000	77.084	1.11	5.24	
ATOM	2320	CA	PRC	563		77.1		31.287	73.794	1.00		
ATOM	2321	CB	PRC	563		78.1		32.376	79.111	1.00	7.10	Many de la companie
MOTA	2322	CG	PRC	563		77.6		23.548	73.404	1.00	5.79	
MOTA	2323	С	PRC	563		75.9		31.277	79.788	1.00	10.73	
MOTA	2324	-0	PRC	563		74.9		32.001	79.558	1.20	11.36	3
MOTA	2325	N	TEP	564		75.9		30.362	80.772	1.00	8.20	-
ATOM	2326	CA	TPP	554		74.9		30.255	81.806	1.00	5.30	•
ATOM	2327	32 22	TEF	564		75.3		29.199	82.845	1.00		
ATOM	2328	CC	TRP	564		74.6		27.886	E2.700	1.00		•
MOTA MOTA	2329 2330		TRF	564 564		73.2		27.585	82.941			3
ATOM	2331		TRP	564 564		73.1		26.188 28.357	82.761 83.296	00		5
ATOM	2332	CDI		564		75.		26.700	82.387	1.00		
	-								J		9.20	

bref21	lc.pd	b		Thu	Apr	25	12	: 27	1:47	1996		31	
ATOM	2333	NE 1	TRP	564		4.33			675	82.422		5.06	-
ATOM	2334	CZ2		564		71.88			546	82.929	1.00	5.49 6.79	₹ ₹
MOTA	2335	CZ3	TRP	564		70.92			723 328	83.461 83.279	1.00	3.18	4
ATOM	2336	CH2		564		70.80 74.81			597	62.525	1.00	5.66	ŧ.
MOTA	2337	č	TRP TRP	564 564		75.9			259	82.740	1.00	9.32	÷
ATOM	233B 2339	O N	LYS	565		73.6			997	82.927	1.00	3.69	7
ATOM ATOM	2340	CA	LYS	565		73.5		33.	256	83.612	1.00	2.00	4
ATOM	2341	CB	LYS	565		73.0	99		332	82.625	1.00	2.00	£
ATOM	2342	CG	LYS	565		74.2			886	81.791	1.00	2.00 3.81	: -{
ATOM	2343	CD	LYS	565		73.8			.197	E0.371 79.711	1.00	3.15	÷
MOTA	2344	CE	LYS	565		74.8			.116 .374	80.497	1.00	6.31	-
MOTA	2345	NZ	LYS LYS	565 565		72.6			.171	84.878	1.00	3.24	<i>₹</i>
ATOM	2346 2347	0	LYS	565		71.8			.270	85.043	1.00	2.93	= -
ATOM ATOM	2348	N	LEU	566		72.8		34	.113	85.783	1.00	3.46	
ATOM	2349	CA	LEU	566		72.1	60		.100	87.042	1.00	6.16	÷ :
MOTA	2350	CB	LEU	566		73.1			.857	88.143	1.00	7.13	ŧ \$
MOTA	2351	CG	LEU	566		72.9			.890	89.641		11.04 13.73	÷
MOTA	2352		LEU	566		74.1			.292	90.343		11.29	
MOTA	2353		LEU	566 566		72.6			.418	87.265	1.00	6.69	4
MOTA	2354	C	LEU	566		72.			.430	87.315	1.00	6.50	
ATOM	2355	C N	CYS	567		70.			.446	£7.406	1.00	7.27	=
MOTA	2356 2357	CA	CYS	567		69.			.738	£7.658	1.00	10.38	₹.
MOTA MOTA	2358	c.	CYS	567		69.	245	27	.013	69.124		13.50	•
ATOM	2359	0	CYS	567		69.			.113	ε9.983		13.64	€
ATOM	2360	CЭ	CYS	567		68.			7.017	86.707		12.07	1.5
ATOM	2361	SG	CYS	567		67.			5.797 3.293	66.808 89.405		15.13	- :
MOTA	2362	N	ARG	568			009 626		3.233			14.78	ē
MOTA	2363	CA	ARG ARG	568 568			781		3.310			17.37	÷
MOTA	2364 2365	CB	ARG	568			037		0.829			20.45	÷
MOTA MOTA	2366		ARG	568			329		0.711		1.00	20.67	÷
MOTA	2367		ARG	568		72.	045		1.996			22.26	7
ATOM	2368		ARG	568			587		2.642			22.85	÷
ATOM	2369	NH	1 ARG	568			531		2.151			20.25	?
ATOM	2370		2 ARG	568			191		3.816			24.23	÷
ATOM	2371		ARG	568			185		8.399 8.690			15.75	Ē
MOTA	2372		ARG	568 569			. 247 . 046		7.752			11.39	-
ATOM	2373 2374		LEU LEU	569			782		7.304				٤
ATOM ATOM	2375			569			.005		6.101				÷
MOTA	237			569			.069		4.91				
ATOM	237		1 LEU	569			.374		4.90				÷
ATOM	237		2 LEU	569			.852		3.67 8.46				•
ATOM	237		LEU				.318		9.22				=
ATOM	238		LEU HIS				.015		38.64				
ATOM	238 238						.454		39.71			0 10.84	
ATOM ATOM	238						.841		40.81	1 93.65		0 11.04	
ATOM	238)		. B2		41.54			0 10.31	
ATOM		5 C	D2 HIS				.73		42.49			0 13.10	
ATOM	238		D1 HIS				. 84		41.42			0 14.30 0 14.17	
ATOM			E1 HIS				.72		42.26 42.92			0 12.65	
ATOM			E2 HIS				2.35		39.07				
ATOM		10 . C					2.09		37.38			0 14.4	} :
ATOM ATOM							1.72		39.86				
ATOM			A GLI				0.65		39.36				
ATOM			B GL	N 57			1.18		38.80			0 11.4	
ATOM	1 239		G GL				0.15		38.01			00 13.0° 00 21.5	
ATON			D GL				0.18 1.16			92 100. 6 37 101.3		00 23.6	
ATON			E1 GL				9.11			62 1C1.1		0C 22.7	
OTA OTA			NE2 GL				9.71		40.5				
ATO			SL				0.09		41.6		85 1.0		
OTA			N AL				8.44		40.1				
ATO			CA AL	A 51			7.34		41.0				
ATO	M 24	02	CR WI		?2		6.92		41.7				
ATO			C AL		72		6.2		40.2				
ATO			O AL		72: 73:		6.2		38.9			00 9.5	
ATO			N PF CD PF		73 73		5.0		42.1			OC 5.4	
ATO ATO			CA PE		73		4.2		39.8			00 F.1	
ATO					73		33.7		40.4	137 100.	596 1.	O().	
ATC			CG PI	P.C 5	73		54.7			99 100.		0(".:	
ATC		10	C PI	RC 5	73	:	53.0	44	39.7	134 93.	317	00 7.1	3

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ATOM	2411	0	PRO	573	52.768	40.608	97.552	1.00 7.72 3
ATOM	2412	N	THR	574	52.428	38.574	98.476	1.00 8.95
ATOM	2413	CA	THR	574	51.255	38.232	97.727	1.00 10.96
ATOM	2414	CB	THE	574	51.075	36.738	97.733	1.00 10.37 6
ATOM	2415	OG1	THE	574	52.135	36.153	96.980	1.00 14.24
ATOM	2416	CG2	THR	574	49.712	36.324	97.155	1.00 13.72 6
ATOM	2417	С	THR	574	50.119	38.852	98.515	1.00 12.85 6
ATOM	2418	0	THR	574	50.163	38.874	99.753	1.00 14.59 3
ATOM	2419	N	ALA	575	49.087	39.324	97.812	1.00 14.88 7
ATOM	2420	CA	ALA	575	47.934	39.946	98.467	1.00 14.50 6
MOTA	2421	CB	ALA	575	46.933	40.433	97.439	1.00 14.72 6
ATOM	2422	С	ALA	575	47.282	38.960	99.443	1.00 14.38 6
ATOM	2423	0	ALA	575	46.480	39.355	100.286	1.00 15.91 3
MOTA	2424	N	ARG	576	47.663	37.695	99.344	1.00 12.79 7
MOTA	2425	CA	ARG	576	47.178		100.189	1.00 11.82 6
ATOM	2426	CB	ARG	576	46.877	35.414	99.328	1.00 15.95 6
ATOM	2427	CG	ARG	576	45.534	35.451	98.604	1.00 20.92 6
ATOM	2428	CD	ARG	576	45.633	34.631	97.302	1.00 24.61 6
ATOM	2429	NE	ARG	576	44.350	34.081	96.848	1.00 27.37 7
ATOM	2430	CZ	ARG	576	44.171	33.438	95.687	1.00 28.99 6
ATOM	2431	NH1		576	45.188	33.261	94.833	1.00 29.46 7
ATOM	2432			576	42.979	32.928	95.391	1.00 27.90 7
ATOM	2433	C	ARG	576	48.090		101.351	1.00 9.90 5
ATOM	2434	0	ARG	576	47.843		101.972	1.00 8.14 8
ATOM	2435	N N	GLY	577	49.167		101.606	1.00 10.36 7
ATOM	2436	CA	GLY	577	50.066		102.705	1.00 9.58 6
ATOM	2437	Ċ	GLY	577	51.201		102.435	1.00 11.02 6
ATOM	2438	0	GLY	577	51.959		103.356	1.00 10.42
ATOM	2439	N	ALA	578	51.263			1.00 11.51 7
ATOM	2440	CA	ALA	578	52.332		100.730	1.00 10.32 6
ATOM	2441	CB	ALA	578	51.842	33.360	99.617	1.00 6.95 5
ATOM	2442	C	ALA	578	53.443		100.212	1.00 10.21 6
ATOM	2443	Ö	ALA	578	53.278		100.138	1.00 9.88 8
ATOM	2444	N	VAL	579	54.597	34.593	99.905	1.00 9.95 7
MOTA	2445	CA	VAL	579	55.673	35.431	99.406	1.00 10.55 6
ATOM	2446	CB	VAL	579	56.957		100.247	1.00 9.32 6
ATOM	2447		VAL	579	56.734		101.618	1.00 8.45 €
ATOM	2448		VAL	579	57.363		100.350	1.00 11.44 6
ATOM	2449	C	VAL	579	55.923	35.128	97.939	1.00 9.09 6
ATOM	2450	0	VAL	579	55.599	34.044	97.452	1.00 8.40 3
ATOM	2451	N	ARG	580	56.460	36.104	97.229	1.00 7.06 7
ATOM	2452	CA	ARG	590	56.721	35.917	95.816	1.00 7.86 6
ATOM	2453	CB	ARG	580	55.769	36.792	94.991	1.00 8.84 6
ATOM	2454	CG	ARG	580	55.926	36.721	93.503	1.00 7.8B 6
ATOM	2455	CD	ARG	580	55.080	37.813	92.844	1.00 B.7B 5
ATOM	2456	NE	ARG	580	53.652	37.517	92.913	1.00 6.85
ATOM	2457	CZ	ARG	580	52.719	38.362	93.341	1.00 5.69 4
ATOM	2458			580 580	53.050	39.581	93.731	1.00 5.12 7
atom atom	2459		ARG		51.470	37.952	93.466	1.00 2.00 7
	2460	C	ARG	580	58.159	36.282	95.523	1.00 7.72 &
ATOM	2461	O N	ARG	580	58.664	37.321	95.954	1.00 7.66 3
ATOM	2462	N Cr	PHE	581 581	58.827 60.200	35.387 35.596	94.827	1.00 6.07 7
atom Atom	2463 2464	CA CB	PHE PHE	581	60.982	34.355	94.458	1.00 5.52 5
ATOM	2465	CG	PHE	581	61.274	34.333	94.803 96.250	1.00 4.84 5 1.00 4.90 5
ATOM	2466		PHE	531	60.510	33.372	97.045	
ATOM	2467		PHE	581	62.371	34.883	96.822	
ATOM	2468		PHE	531	60.835	33.191	98.390	
ATOM	2469		PHE	581	62.694	34.700	98.165	1.00 4.44 5
ATOM	2470	CZ	PHE	581	61.926	33.854		1.00 5.88 6 1.00 3.43 6 1.00 5.46 6 1.00 6.33 8 1.00 6.16 7
ATOM	2471	C	PHE	531	60.287		98.944	1.00 3.43 6
ATOM	2472	5	PHE	581	59.686	35.939 35.101	92.961 92.194	1.00 5.46 6
ATOM	2473	N	TRP	582	61.037			1.00 6.33 8
ATOM				532	61.129	26.844	92.525	00 5.16 7
	2474	CA	TRP			37.054	91.090	1.00 7.26 6
aton: Atom	2475 2476	CB	TRP	582 582	59.861 59.463	37.773	90.589	1.00 7.26 6 1.00 9.34 5 1.00 10.74 6 1.00 11.49 5 1.00 11.22 6
ATOM	2477	CDS	TRP TRP	532	59.462	38.933	91.423	1.00 10.74
ATOM				582	59.916	40.268		1.00 11.49
	2478		TEP	582	59.366	41.017		1.00 11.22
ATOM ATOM	2479		TPP	532	60.744	40.906		1.00 11.65 6 1.00 14.19 6 1.00 12.18
ATOM	2480 2481		TPP	582	58.663	28.915		1.00 14.19 4
ATOM	2481		TRP	532 532	58.604	40.165		1.00 12.18
ATOM	2482	CZZ		582	59.618	42.365		1.00 12.31
ATOM	2484	CH		582	61.001	42.247		1.00 15.91
ATOM	2485	0	TP.P	592 582	60.436	12.973		1.00 16.33
ATOM	2485	ó	TPP	582	62.409	37.522		1.00 7.94
ATOM	2487	N	CYS	583	63.219 62.55€	38.299		1.00 5.37
ATOM	2488	CA	CYS	583	62.55e	37.312 37.766		00 7.90
0.7	00		- 1 -	505	95.056	-,./00	00.334	1.0(9.15 8

bref2	lc.pd	b		•	Thu	Apı	25	12	:27	:47	19	96			33	
ATOM	2489	С	CYS	5	93		63.15	4	38.	449	٤?.	073	1.00		52	÷
ATOM	2490	õ	CYS		83		62.14		38.		86.		1.00		13	3 6
MOTA	2491	CB	CYS	5	83		64.50		36.			876	1.00			9 1 6
ATOM	2492	SG	CYS		183		65.60		36.			470	1.00			7
ATOM	2493	N	SER		84		63.89			453		606 375	1.00			÷
MOTA	2494	CA	SER		84		63.55			150 612		649	1.00			Ś
MOTA	2495	CB	SEP		584		63.23			141		680	1.00			3
ATOM	2496	oG	SER		584		64.8			052		531	1.00			5
MOTA	2497	Ç	SER		584 584		65.8			485		990	1.00			3
ATOM	2498	o N	SER		585		64.7			357		390	1.00	8	.82	7
MOTA	2499 2500	CA	LEU		585		65.8			214	٤2.	.500	1.00		.31	ē
MOTA MOTA	2501	CB	LEU		585		65.6	38	38.	192		. 374	1.00		. 24	÷
ATOM	2502	cs	LEU		585		65.2	65		. 731		.541	1.00		.00	6
ATOM	2503	CD1	LEU		585		65.9			.888		.486	1.00	_	.00	6 5
ATOM	2504	CD2	LE		585		65.6			.271		.912 .832	1.00		.79	5
MOTA	2505	C	LE		585		66.1			.562 .282		.508	1.00		.56	á
MOTA	2506	0	LE		585		65.1 67. 4			.929		.637			.50	7
ATOM	2507	N	PRO		586 586		68.6			.279		.160			.29	6
MOTA	2508	CD	PR		586		67.7			.202		.993			.85	ક
ATOM	2509 2510	CB	PR		586		69.2			.304	٤1	.191	1.0	0 11	1.45	ó
ATOM ATOM	2511	cG	PR		596		69.5		41	.470	82	.416	1.0	0 13	3.83	5
MOTA	2512	c	PR		586		67.4	116	42	.019		.520			4.14	6
MOTA	2513	ō	PR		586		67.6			.019		.912			4.17	5 7
ATOM	2514	N	TH	R	587		66.			.985		. 957			3.17	ŕ
MOTA	2515	CA	TH		587		66.2			.949		.569			2.49 5.17	6
ATOM	2516	CB	TH		587		66.			.355		3.969 3.002			8.67	8
ATOM	2517		1 TH		587		65.			.330		5.929			7.05	6
ATOM	2518	CG			587		65.67.			2.186		5.657			2.00	6
MOTA	2519	C	TH		587 587		66.			.308		5.948			1.83	9
MOTA	2520 2521	O N	Al		588		68.			2.530		6.700	1.0	00 1	1.51	7
MOTA MOTA	2522	CA			588		69.			1.927	7.	5.849	1.0	00	7.86	ó
ATOM	2523				588		70.	896	4:	2.342	7.	6.320			8.95	6
ATOM	2524		Al		588		69.	435	41	0.425		5.700			7.36	న
ATOM	2525		AI	LA	588		69.			9.894		4.681			8.37	ā
MOTA	252€		A:		589			877		9.747		6.693			7.82	7 5
MOTA	2527			SP	589			745		8.300	_	6.651 7.976			7.85 5.24	6
MOTA	2528			SP	589			173		7.684 7.683		3.168			5.26	5
ATOM	2529			SP	589			673 088		8.045	_	9.298			6.38	9
ATOM	2530)1 A)2 A		589 589			42		7.299		7.230		00	2.00	
ATOM	2533 2533			SP	589			34		7.845		5.376		00	7.96	:
ATOM ATOM	253			SP	589			. 08		6.659	_	5.383	3 1.	00	7.86	
ATOM	253			HF.	590		66	. 43	5 3	8.780		5.13		00	8.88	
ATOM	253		L T	HF.	590)		. 04		8.45		5.89			10.02	
ATOM	253	6 C	5 T	HP	590)		. 11		9.57	_	5.42		00	8.46	
MOTA	253			HF.	590			. 49		0.80		5.84		00	7.66 10.59	
ATOM			52 I		590			. 26		9.72		7.92 74.46			10.88	
ATOM			_	HR	590 590			.69 .61		38.10 38.41		74.00			15.28	_
ATOM				HF. EF.	591			.59		37.40		73.78			11.68	
ATOM ATOM				ER	593			.37		37.02		72.39	1 1.		11.91	. 5
ATOM				SER	593		66	. 69	2	36.68		71.69			13.98	3 -
ATOM				SEP.	59		67	. 04	6	37.71		73.79			16.79	
MOTA			: :	SER	59	1		.40		35.86		72.17			11.54	
ATOM		16 · C		SER	59			. 45		34.84		72.88 71.13		.00	9.3	
4OTA				SEF.	59			.58		35.99		70.80		.00	5.8	
MOTA				SEP.	59 59			39		34.98 35.63		30.11		.00	5.2	
ATON				SER. Ser	59			7		36.63		70.91		.00	5.4	
1OTA				SER	59			3.2		33.94		€9.88		.00	5.3	
ATO				SEF.	59			1.3		33.9		69.56		.00	4.7	
OTA OTA				PHE	59			2.3		32.98		€9.5	37 1	.00	5.7	9 7
ATO				PHE	59		63	2.7	15	31.90	00	€3.6	20 1	.00	8.3	
ATO				PHE	59			2.8		32.4		€7.1		. 00	7.5	
ATO		56	CG	PHE	5 3			1.7		33.4		£5.7		00	5.7	
ATO	M 25	57	CD1		59			2.0		34.6		£5.1		00 aa	9.2	
ATO			CD2		53			0.3		33.1		67.0 65.8		oc		
ATO			CEI		59			1.0		35.5 34.0		65.7		. 50		
ATO			CE2			93 33		9.3 9.6		35.2		55.1		00		
ATO			22	PHE		93 93		3.8		30.9		69.0		1.00		
ATC ATC		62 63	C 5	PHE		93		4.3		30.1		63.1			11.0	
ATC		64	N	VAL		94		4.2		30.9		70.2		1.00	9.3	32
ATC		65	CA	VAL		94	€	5.2	84	30.1	13	70.9		1.00		
ATC		66	CF	IAV		94	é	6. :	98	30.9	909	71.1	.55	00	9.	17

bref2	lc.pd	Ъ		Thu	Apr 25 1	2:27:47	1996	34	ŀ
ATOM	2567	CG1	VAL	594	67.086	31.490	69.894	1.00 11.27	1
ATOM	2568		VAL	594	66.359	32.005	72.175		
ATOM	2569	C	VAL	594	64.874			1.00 3.98	
						29.552	72.261	1.00 6.86	
ATOM	2570	5	VAL	594	64.201	30.239	73.037	1.00 9.44	
MOTA	2571	N.	PRO	595	65.287	28.308	72.572	1.00 4.06	
ATOM	2572	CD	PRO	595	65.910	27.414	71.592	1.00 4.50	·
ATOM	2573	CA	PRO	595	65.040	27. 5 58	73.802	1.00 4.33	·
ATOM	2574	CB	PRO	595	65.623	26.185	73.468	1.00 4.07	•
ATOM	2575	CG	PRO	59 5	65.442	26.084	72.064	1.00 2.00	£
ATOM	2576	С	PRO	595	65.728	28.142	75.048	1.00 3.58	
ATOM	2577	0	PRO	595	66.955	28.077	75.180	1.00 3.03	
MOTA	257B	N	LEU	596	64.923	28.692	75.955	1.00 3.21	
MOTA	2579	CA	LEU	596	65.420	29.282	77.199	1.00 4.16	
ATOM	2580	CB	LEU	596	64.670	30.596	77.561	1.00 3.29	
ATOM	2581	CS	LEU	596	65.384	31.870	78.068		
			LEU	596	64.500			1.00 2.00	
ATOM	2582					32.639	79.002	1.00 3.47	
ATOM	2583		LEU	596	66.646	31.534	78.783	1.00 2.16	
ATOM	2584	С	LEU	596	65.252	28.293	78.347	1.00 4.67	
ATOM	2585	0	LEU	596	64.121	27.938	73.721	1.00 2.52	
ATOM	2586	N	GLU	597	66.384	27.861	78.900	1.00 4.53	,
MOTA	2587	CA	GLU	597	66.406	26.943	80.031	1.00 3.76	
ATOM	2588	CB	GLU	597	67.566	25.980	79.909	1.00 2.00) =
ATOM	2589	CG	GLU	597	67.699	25.125	81.113	1.00 2.00)
ATOM	2590	CD	GLU	597	68.548	23.955	80.855	1.00 5.62	
ATOM	2591	OE 1	GLU	597	69.206	23.971	79.805	1.00 10.01	
ATOM	2592	OE 2	GLU	597	68.562	23.014	81.675	1.00 6.65	
ATOM	2593	С	SLU	597	66.483	27.704	81.367	1.00 2.57	
MOTA	2594	Ö	GLU	597	67.322	28.596	81.536	1.00 3.19	
ATOM	2595	N	LEU	598	65.590	27.35B	82.296	1.00 3.03	
ATOM	2596	CA	LEU	598	65.519	28.001	£3.600	1.00 2.16	
ATOM	2597	CB	LEU	598	64.159	28.670	83.777	1.00 2.10	
ATOM	2598	CG	LEU	598	63.756	29.657	82.681		
ATOM	2599		LEU	598	62.279	29.702		1.00 2.00	
							82.601	1.00 2.00	
MOTA	2600		LEU	598	64.368	31.027	82.888	1.00 2.00	
ATOM	2601	C	LEU	59B	65.761	26.988	64.700	1.00 2.92	
ATOM	2602	0	LEU	598	65.337	25.833	84.605	1.00 2.64	
ATOM	2603	N	ARG	599	66.462	27.428	85.736	1.00 2.34	
ATOM	2604	CA	ARG	599	66.804	26.580	86.862	1.00 3.62	<u> </u>
ATOM	2605	CB	ARG	599	68.254	26.115	86.710	1.00 6.78	3 - 5
ATOM	2606	CG	ARG	599	68 .4 79	24.611	86.512	1.00 10.90) :
ATOM	2607	CD	ARG	599	69.385	24.359	85.308	1.00 14.84	1 ÷
ATOM	2608	NE	ARG	599	69.658	22.945	85.047	1.00 17.19	1 = = = = = = = = = = = = = = = = = = =
MOTA	2609	CZ	ARG	599	70.176	22.100	€5.942	1.00 17.80) ÷
ATOM	2610	NH 1	AP.G	599	70.472	22.515	87.182	1.00 17.23	3 -
ATOM	2611	NH2	ARG	599	70.452	20.845	85.580	1.00 15.70) -
ATOM	2612	С	ARG	599	66.717	27.367	88.150	1.00 3.41	1 1
ATOM	2513	Э	ARG	599	67.394	28.364	68.259	1.00 4.2	
ATOM	2614	N	VAL	600	65.843	26.379	89.081	1.00 2.8	
ATOM	2615	CA	741	600	65.756	27.644	90.387	1.00 2.0	
ATOM	2616	CB	7AL	600	64.322	28.001	90.825	1.00 2.00	
ATOM	2617	CG1		600	64.336	28.512	\$2.248	1.00 2.00	
ATOM	2618		VAL	600	63.737	29.035	89.917		
ATOM	2619	c	VAL	600	66.273	26.622			
					65.744		91.371	1.00 3.2	
ATOM	2620	0	VAL	600		25.525	91.426	1.00 4.1	
ATOM	2621	N	THE	601	67.309	26.963	92.124	1.00 5.2	_
MOTA	2622	CA	THE	601	67.881	26.043	93.098	1.00 6.7	
MOTA	2623	CB	THP.	601	69.296	25.601	92.688	1.00 8.5	0 -
ATOM	2624	· 0G1		601	69.228	24.939	91.430	1.00 12.7	0 £ 7 £ 0 £
MOTA	2625		THE	601	69.890	24.631	93.684	1.30 8.7	
MOTA	2626	C	IHP.	601	67.995	26.634	94.481	1.00 8.7	4 :
MOTA	2627	Ō	THR	601	68.267	27.822	94.637	1.00 11.7	7 -
ATOM	2628	N	ALA	602	67. 78 8	25.792	95.484	1.00 9.8	7 -
MOTA	2629	CA	ALA	602	67.915	25.196	96.877	1.00 9.6	2 :
ATOM	2630	CB	ALA	602	67.254	25.191	97.745	1.00 9.5	
ATOM	2631	C	ALA	602	69.404	26.180	97.153	1.00 10.3	
MOTA	2632	C:	ALA	602	70.107		96.613	1.33 11.8	•
ATOM	2633	N	ALA	603	69.872		93.036	1.00 9.7	
ATOM	2634	CA	ALA	503	71.292		98.415	1.00 7.2	-
ATOM	2635	CB	ALA	603	71.517		99.300	1.00 6.7	
ATOM	2636	2	ALA	603	73.871		99.070	1.00 6.7	3
ATOM	2637	Ş	ALA	603	73.066		99.320	1.00 4.9	
ATOM	2638	N	SER	604	71.026		99.324	1.00 5.8	
ATOM	2639	CA	SER	604	71.497		99.897		
ATOM	2640	CB	SER	604	70.409		100.740	1.00 5.8 1.00 7.4 1.00 5.3	•
ATOM	2641			604	69.702			1.00 5.3	
MOTA	2642	೦೦	SER				99.997	1.00 5.4	
ATOM		C	SER	604	71.914		98.777		
	2643	0	SER	604	72.462		99.042	1.00 11.6	
MOTA	2644	N	31.	605	71.604	23.070	97.535	1.01 }.2	Ġ.

bref2	Lc.pdl	•		Thu	Apr	25	12	: 2	7:47	1996		35	
ATOM	2645	CA	GLY	605		71.9			262	96.378			ŧ
ATOM	2646		GLY	605		70.7			620	95.785			
MOTA	2647	0	GLY	605		70.7			198	94.631	-	8.81 7.11	-
ATOM	2648	N	ALA	606		69.6			.606 .001	96.573 96.194		6.20	:
ATOM	2649	CA	ALA	606		68.3 67.4			.885	97.387		2.64	=
ATOM	2650	CB	ALA ALA	606 606		67.6			.770	95.113		6.88	÷
ATOM	2 6 51 2652	0	ALA	60 e.		67.4			. 974	95.234		7.80	-
ATOM ATOM	2653	N	PRO	607		67.2			.063	94.074	1.00	6.21	
MOTA	2654	CD	PRO	607		67.4	57		.636	93.821	1.00	6.78	1
ATOM	2655	CA	PRO	607		66.5			.660	92.950	1.00	7.75 7.27	ŧ .
ATOM	2656	CB	PRO	607		66.6			.587	91.845 92.355	1.00	5.40	ŧ
ATOM	2657	ÇG	PRO	607		67.6			.620 .969	93.220	1.00	6.86	
MOTA	2658	0	PRO PRO	607 607		64.2			.084	93.599	1.00	6.25	=
MOTA MOTA	2659 2660	и	ARG	608		64.			.215	92.953	1.00	6.55	-
MOTA	2661	CA	ARG	608		63.2	284	23	.658	93.095	1.00	6.82	1
ATOM	2662	CB	ARG	608		63.			.105	93.591	1.00	7.55	ŧ.
ATOM	2663	ÇG	ARG	608		63.			.320	95.066	1.00		
MOTA	2664	CD	ARG	608		62.			.474	95.992 95.820	1.00		
MOTA	2665	NE	ARG	608		61. 60.			.719 5.828	96.200	1.00		- - -
MOTA	2666	CZ	ARG	608 608		61.			5.817	96.773	1.00		-
MOTA	2667 2668		ARG	608			218	-	5.936	96.048	1.00	13.38	-
ATOM ATOM	2669	C	ARG	608			586		3.548	91.739	1.00	6.91	÷
ATOM	2670	Ö	ARG	608		61.	613	2:	2.836	91.612	1.00	9.99	-
ATOM	2671	51	TYP	609			095		4.194	90.700	1.00	7.03	,
ATOM	2672	CA	TYP.	609			405		4.140	89.406	1.00	7.82	₹ -
MOTA	2673	CB	TYP.	609			533		5.394	89.203 90.298	1.00	9.92 11.75	
ATOM	2674	Ç.C	TYP	609			543 700		5.684 6.798	91.137		12.36	ŧ
MOTA	2675	CD:	I TYR I TYR	609 609			768		7.078	92.156		13.98	₹.
ATOM	2676 2677		2 TYR	609			434		4.852	90.499		13.86	÷
MOTA MOTA	2678		2 TYP.	609			494		5.120	91.506		13.63	-
ATOM	2679		TYP.	609		58.	664		6.235			15.21	:
MOTA	2680		TYF.	609			. 689		6.529			17.36	÷
ATOM	2681	Ç	TYP.	609			. 316		4.032			7.45 10.10	
MOTA	2682		TYR	609			.448		4.514 3.416			4.17	:
ATOM	2683		HIS	610			.803 .536		3.308			3.51	÷
ATOM	2684			610 610			.306		1.995			2.85	Ē
MOTA MOTA	2685 2686			610			.112		1.883			2.00	÷
ATOM	2687		2 HIS	610		65	. 692	: 2	22.830	83.75		2.00	<u>:</u>
ATOM	2688		1 HIS	610		65	.346		20.681			2.00	
MOTA	2689	CE	1 HIS	610			.030		20.893				:
ATOM	2690		2 HIS	610			. 250		22.189 23.456				•
MOTA	2691		HIS	610 610			.500		22.824				÷
ATOM	2692 2693		HIS ARG				. 79	5	24.30				•
ATOM ATOM	269						. 85		24.56		6 1.00		:
MOTA						60	. 94		25.70				•
ATOM						5 9	. 47		25.57				- 1
ATOM							3.70		26.89				=
ATOM							7.50 6.64		26.83 27.83				2
ATOM							6.85		28.97				į
ATOM			H1 ARC H2 A RC				5.60		27.71				-
ATOM ATOM							2.65		24.99		8 1.00	2.00	:
ATOM							3.80		25.35	0 21.68			-
ATOM							2.07		24.33				
ATOM		5 2	A VA				2.66		25.25				:
4OTA			B VA				3.05		24.06				
OTA			G1 VA				3.80 3.91		24.56				
ATOPA .			G2 VA				1.49		25.96				
ATO							0.31		25.43				:
ATO:			I IL				1.6		27.16	77.9	68 1.0	0 2.39	
ATO			A IL			ŧ	0.5	57	27.3				
ATO			B IL				9.8		28.9				
OTA	M 27:	14 3	CG2 IL				9.2		28.2				,
ATO			CG1 IL		13		50.8		30.0				
ATO			CD1 II C II		13 13		50.2 50.9		28.5				
OTA OTA			o II O II		13		52.1		28.5		09 1.0	e 2.06	
ATO			N HE		14		50.0		29.1	73 75.4	12 1.0	00 3.35	
ATO			CA H	s 6	14		60.2	52	30.0				
ATC	M 27	21	CB H		14		59.6		29.4				
ATC	M 27	22	CC H	15 6	14		ć(ı.4	4 7	28.4	10 72.2	271 1.4	30 2.10	~

bref2	1c.p	i b		Thu	Apr 25	12:27:47	1996	36
ATOM	2723	CD2	HIS	614	61.353	28.536	71.281	1.00 2.96 ÷
ATOM	2724		HIS	614	60.442		72.609	1.00 2.96 £ 1.00 4.63 7
ATOM	2725		HIS	614	61.310		71.865	1.00 2.00 5
ATOM	2726	NE2	HIS	614	61.875		71.051	1.00 6.31 7
ATOM	2727	С	HIS	614	59.580		74.664	1.00 3.58 5
ATOM	2728	<u>ې</u>	HIS	614	58.419		75.046	1.00 2.50 3
ATOM	2729	N	ILE	615	60.315	32.412	74.674	1.00 2.76 7
ATOM	2730	CA	ILE	615	59.717	33.661	75.108	1.00 2.55 6
ATOM	2731	CB	ILE	615	60.770	34.768	75.221	1.00 2.49 5
ATOM	2732		ILE	615	60.102		75.507	1.00 2.99 4
ATOM	2733	CG1	ILE	615	61.785		76.307	1.00 2.00 6
ATOM	2734	CD1	ILE	615	63.067		76.351	1.00 2.00 6
ATOM	2735	C	ILE	615	58.569		74.205	1.00 3.27 5
ATOM	2736	0	ILE	615	57.609		74.651	1.00 5.04 3
ATOM	2737	N	ASN	616	58.639		72.943	1.00 5.73 7
ATOM ATOM	2738 2739	CA CB	ASN ASN	616 6 16	57.618		71.945	1.00 4.76 6
ATOM	2740	CG	ASN	616	58.205 58.860		70.513	1.00 2.00 6
ATOM	2741		ASN	616	58.410		70.236 69.399	1.00 2.00 6
ATOM	2742		ASN	616	59.954		70.910	1.00 2.00 3 1.00 2.00 7
ATOM	2743	С	ASN	616	56.287		72.124	1.00 2.00 7 1.00 4.60 5
ATOM	2744	0	ASN	616	55.265		71.581	1.00 4.00 3
ATOM	2745	N	GLU	617	56.280		72.989	1.00 4.63 7
ATOM	2746	CA	GLU	617	55.088		73.242	1.00 5.16 6
ATOM	2747	CB	GLU	617	55.424		73.185	1.00 4.92 6
MOTA	2748	CG	GLU	617	56.381		72.086	1.00 8.53 6
ATOM	2749	CD	GLU	617	56.433		71.704	1.00 11.83 6
ATOM	2750	CE1	GLU	617	56.653		70.498	1.00 15.40 3
MOTA	2751	SE2	GLU	617	56.27€	27.297	72.575	1.00 14.68 3
ATOM	2752	С	GLU	617	54.438	31.744	74.587	1.00 4.18 5
ATOM	2753	3	GLU	617	53.440	31.127	74.930	1.00 7.74 9
ATOM	2754	N	VAL	618	54.995		75.354	1.00 3.63 7
ATOM	2755	CA	VAL	618	54.433		7 6.65 5	1.00 2.00 6
ATOM	2756	CB	VAL	618	55.365		77.870	1.00 2.00 6
ATOM	2757	CG1	VAL	618	55.666		77.838	1.00 2.00 6
ATOM	2758		VAL	618	56.651		77.890	1.00 2.00 6
ATOM ATOM	2759 2760	C O	VAL	618	54.119		76.727	1.00 2.00 6
ATOM	2761	N	VAL VAL	618	54.600		77.616	1.00 2.77 3
ATOM	2762	CA	VAL	619 619	53.333 52.970		75.778	1.00 2.00 7
ATOM	2763	СВ	VAL	619	52.76		75.792	1.00 3.10 6
ATOM	2764		VAL	619	52.743		74.407 74.449	1.00 2.32 6
ATOM	2765		VAL	619	53.884		73.519	1.00 2.43 5 1.00 7.61 6
ATOM	2766	ε	VAL	519	51.700		76.589	1.00 7.61 6 1.00 4.11 6
ATOM	2767	0	VAL	619	50.81		76.610	1.00 6.41 3
ATOM	276B	N	LEU	620	51.639		77.268	1.00 2.53 7
ATOM	2769	CA	LEU	620	50.492		78.080	1.00 3.37 6
ATOM	2770	CB	LEU	620	50.702		79.554	1.00 3.89 6
ATOM	2771	CG	LEU	620	49.613	37.183	80.438	1.00 3.95 6
ATOM	2772	CD1	LEU	520	50.233	37.141	81.775	1.00 5.62 6
MOTA	2773	CD2	LEU	620	48.30	37.985	80.529	1.00 3.31 6
MOTA	2774	C	LEU	620	50.3B		77.920	1.00 5.44 -
ATOM	2775	٥	LEU	620	50.858		78.736	1.00 7.07 a
ATOM	2776	N	LEU	621	49.73		76.834	1.00 7.07 7
MOTA	2777	CA	LEU	621	49.54		76.465	1.00 5.70 6
ATOM	2778	CB	LEU	621	48.83		75.111	1.00 5.58 6
ATCM ATOM	2779 2780	· CD1	LEU	621	49.46		73.845	1.00 2.00 5
ATOM	2781		LEU	621	48.39		72.831	1.00 2.42 6
ATOM	2782	C	LEU	621 621	50.545 48.736		73.377	1.00 2.00 6
ATOM	2783	5	LEU	621	47.94		77.427	1.00 7.59 6
ATOM	2784	N.	ASP	622	48.921		78.198	1.00 8.04 3
ATOM	2785	CA	ASP	622	48.14		77.355 78.128	1.00 11.43 7 1.00 10.55 6
ATOM	2786	CB	ASP	622	48.67		77.968	
ATOM	2787	26	ASP	522	49.74		73.963	1.00 9.98 5
ATOM	2788		ASF	622	50.39		78.724	1.00 11.16 5 1.00 12.42 3
ATOM	2789		ASF	622	49.92		79.976	1.00 12.42 5
ATOM	2790	0	ASF	622	46.85		77.336	1.00 11.12
ATOM	2791	5	ASP	622	46.86		76.152	1.00 11.16 3
ATOM	2792	23	ALA	623	45.75		77.965	7.00 13.11
ATOM	2793	SA	ALA	623	44.45		77.326	1.00 12.49 6
ATOM	2794	CB	ALA	623	43.37		78.402	1.00 13.24 5
MOTA	2795	3	ALA	523	44.26		75.399	1.00 10.77 6
MOTA	2796	2,	ALA	523	45.01	3 46.953	76.489	1.00 11.45 3
ATOM	2797	N	PRO	624	43.31		75.462	1.00 7.62 7
ATOM	2798	CD	PRC	624	42.60		75.175	1.00 7.09 6
ATOM	2799	CA	PP.C	624	42.96		74.486	1.00 6.69 6
ATOM	2800	CF	PRO	624	41.93	3 46.241	73.632	.00 6.32 6

bref21	lc.pd	ь		Thu A	pr 25	12:2	7:47	1996	37
ATOM	2801	ÇG	PRO	624	42.33			73.736 75.095	1.00 9.96 5 1.00 10.98 5
ATOM	2802	С	PRO	624	42.36			76.056	1.00 13.90
ATOM	2803	0	PRO	624	41.59	_	.352	74.518	1.00 11.27
ATOM	2804	N	VAL VAL	625 625	42.15		.638	74.969	1.00 8.57 5
ATOM	2805 2806	CA CB	VAL	625	43.25		.676	75.160	1.00 8.17
ATOM ATOM	2807		VAL	625	44.09		324	76.386	1.00 10.17 5
ATOM	2808	CG2	VAL	625	44.1		.744	73.933	1.00 6.41 6
MOTA	2809	C	VAL	625	41.1		1.193	73.950 72.970	1.00 11.35
ATOM	2810	O	VAL	625	40.7		0.513 2.392	74.243	1.00 10.53
MOTA	2811	Ŋ	GLY	626 626	40.6 39.6		3.098	73.389	1.00 12.11
ATOM	2812	CA	GLY GLY	626	38.3		2.482	72.843	1.00 14.18
MOTA	2813	3	GLY	626	37.9	_	2.907	71.775	1.00 14.32
ATOM	2814 2815	N	LEU	627	37.8		1.522	73.565	1.00 16.36
ATOM ATOM	2816	CA	LEU	627	36.5		0.879	73.112	1.00 17.03 6
ATOM	2817	CB	LEU	627	36.1		9.789	74.092	1.00 13.89 5 1.00 13.26 5
ATOM	2818	CG	LEU	627	34.9		8.955	73.631	1.00 15.73
MOTA	2819		LEU	627	35.3		8.124 8.034	74.740	1.00 12.93 6
MOTA	2820		LEU	627	34.4 35.4		1.869	72.92B	1.00 18.27 5
MOTA	2821	ç	LEU LEU	627 627	35.0		2.548	73.881	1.00 17.62 3
ATOM	2822	C N	VAL	628	34.9		2.005	71.682	1.00 19.54
ATOM	2823 2824	CA	VAL	628	33.1		2.862	71.355	1.00 19.76
MOTA MOTA	2825	CB	VAL	628	34.		4.119	70.490	1.00 18.01 6
MOTA	2826		1 VAL	628	34.		55.151	71.318	1.00 19.05
ATOM	2827		2 VAL	628	34.		53.723	69.244	1.00 18.46 f 1.00 21.37 f
ATOM	2828		JAV	628	32.		52.009	70.609	
ATOM	2829		VAL	628	33.		51.171 52.157	€9.740 71.036	
MOTA	2830		ALA	629			51.453	70.440	
ATOM	2831			629 629			50.850		
ATOM	2832		ALA ALA	629			52.496		1.00 22.67
ATOM	2833 2834		ALA	629			53.693	69.980	
ATOM ATOM	2835		ARG	630	28.	823	52.061		
ATOM	283			630		014	52.979		
MOTA	283			630		873	53.703		
ATOM	283	B CC	ARG	630		.087	55.154		
ATOM	283			630		. 565	56.016		
ATOM	284			630		. 366 . 627	58.112		· - · · · · · · · · · · · · · · · · · ·
MOTA	284		Z ARG H1 ARG	630 630		.108	57.460		5 1.00 26.78 7
ATOM	284 284		H2 ARG			.421	59.440		6 1.00 25.78
MOTA MOTA	284		ARG		26	.867	52.308	8 67.12	
MOTA	284					. 945	51.13		
ATOM	284					.787	53.04		· · · · · · · · · · · · · · · · · · ·
ATOM			A LEU			.650	52.49 53.26		
ATOM			B LEC			.379	52.40		
ATOM			G LEU			.275	50.96		1 1.00 18.01 5
ATOM		-	D2 LEG			.351	52.32	_	0 1.00 18.08 6
MOTA						.826	52.77	0 64.79	1 1.00 21.02 5
ATOM ATOM					24	1.739	53.91		
ATOM						.094	51.75		7 1.00 21.42 7
ATOM			A AL			5.170	51.97		
ATON		56 3	B AL			5.601	50.69		
ATON			AL.			3.771	52.42 51.60		
ATON		-	AL			2.964 3.542	53.70		
ATO			N AS		_	2.239	54.3		
ATO			CA AS CB AS	_	_	2.438	55.88		13 1.00 90.00 5
ATO: ATO			CG AS			2.352	56.7	75 63.2	
ATO			OD1 AS			1.778	56.3		
ATO			OD2 AS			2.852	57.9		
ATO			C AS			1.466			
OTA	M 28	66	D AS			0.253	53.6		
ATO			N GI		_	2.137			
ATO		668	CA GI			2.349			
ATO		369 370	CB GI	ມນ 634 ມນ 634	-	22.847			
ATC ATC		370 371		LU 63		23.766			150 1.00 90.00
ATC		872	DE1 G		-	24.012		25 55.	
ATO		873	DE2 G		4 :	24.295	55.6		
ATO		874		LU 63	4 :	20.911			
ATO	OM 2	875	○ G	LU 63		20.024			
AT(876		ER 63		21.46			
ATO		877		ER 63 ER 63		21.062 22.28		_	
TA	um 2	878	CB S	ER 63	-				

bref2	1c.pc	i b		Thu	Apr 25 1	.2:27:47	1996	38
MOTA	2879	OG	SEP.	635	23.189	49.037	60.063	1.00 90.00 3
ATOM	2880	С	SER	635	20.328	49.370	60.435	1.00 90.00 5
ATOM	2881	0	SER	635	19.394	48.552	60.437	1.00 90.00 3
ATOM	2882	N	GLY	636	20.780	50.010	61.488	1.00 90.00 7
ATOM	2883	CA	GLY	636	20.217	49.834	62.821	1.00 90.00 8
MOTA	2884	С	GLY	636	20.996	48.771	63.586	1.00 90.00 5
MOTA	2885	0	GLY	636	20.541	47.640	63.790	1.00 90.00 8
ATOM	2886	N	HIS	637	22.203	49.107	64.010	1.00 29.39 7
ATOM	2887	CA	HIS	637	22.920	48.155	64.847	1.00 28.30 €
ATOM	2888	CB	HIS	637	23.190	46.817	64.148	1.00 27.49 5
MOTA	2889	CG	HIS	637	23.915	46.854	62.796	1.00 26.32 &
MOTA	2890		HIS	637	25.124	47.337	62.400	1.00 26.14 5
ATOM	2891		HIS	637	23.338	46.289	61.665	1.00 26.56 7
MOTA	2892		HIS	637	24.176	46.428	60.659	1.00 26.93 6
ATOM	2893 2894		HIS	637	25.247	47.050	61.079	1.00 26.35 7
ATOM ATOM	2895	0	HIS HIS	637 637	24.223	48.651	65.427	1.00 27.39 6
ATOM	2896	N	VAL	638	24.505 24.921	49.862	65.452	1.00 27.46 3
ATOM	2897	CA	VAL	638	26.119	47.631 47.770	65.868	1.00 25.98 7
ATOM	2898	CB	VAL	638	26.169	46.693	66.646	1.00 22.67 5
ATOM	2899		VAL	638	26.966	47.127		1.00 23.93 6
ATOM	2900		VAL	638	24.781	46.310	68.963 68.251	1.00 24.68 5 1.00 23.20 5
ATOM	2901	c	VAL	638	27.422	47.694	65.877	1.00 23.20 5 1.00 21.16 5
ATOM	2902	Ō	VAL	638	27.763	46.687	65.236	1.00 17.80 B
ATOM	2903	N	VAL	639	28.129	48.808	65.940	
ATOM	2904	CA	VAL	639	29.417	48.927	65.309	
ATOM	2905	СВ	VAL	639	29.362	49.967	64.127	1.00 21.49 f 1.00 22.97 f
ATOM	2906		VAL	639	30.383	51.140	64.296	
ATOM	2907		VAL	639	29.531	49.189	62.796	1.00 22.32 5 1.00 21.09 5
ATOM	2908	С	VAL	639	30.503	49.131	66.402	1.00 18.72 6
ATOM	2909	ō	VAL	639	30.569	50.164	67.103	1.00 15.61 3
ATOM	2910	N	LEU	640	31.245	48.035	66.588	1.00 13.61 3
ATOM	2911	CA	LEU	640	32.312	47.853	67.567	1.00 17.29 7
ATOM	2912	CB	LEU	640	32.296	46.385	69.002	1.00 13.07 6
ATOM	2913	CG	LEU	640	31.948	45.925	69.398	1.00 9.33 6
ATOM	2914		LEU	640	30.755	46.635	69.940	1.00 6.96 5
MOTA	2915		LEU	640	31.703	44.456	69.328	1.00 7.60 5
ATOM	2916	С	LEU	640	33.727	48.158	67.106	1.00 15.19 6
ATOM	2917	0	LEU	640	34.319	47.345	66.393	1.00 13.52
ATOM	2918	N	ARG	641	34.320	49.236	67.616	1.00 15.40 7
ATOM	2919	CA	ARG	641	35.717	49.564	67.269	1.00 18.02 6
ATOM	2920	CB	ARG	641	35.744	50.820	66.406	1.00 18.96 6
MOTA	2921	CG	ARG	641	36.505	50.608	65.100	1.00 23.80 5
ATOM	2922	CD	ARG	641	35.742	51.114	63.884	1.00 25.92 5
ATOM	2923	NE	ARG	641	34.649	50.212	63.502	1.00 26.12 7
MOTA	2924	CZ	ARG	641	33.446	50.620	63.085	1.00 27.21 6
ATOM	2925	NH1	ARG	641	33.173	51.935	63.013	1.00 24.02
ATOM	2926	NH2	ARG	641	32.538	49.716	62.685	1.00 23.76
MOTA	2927	C	ARG	641	36.638	49.707	68.527	1.00 17.87 6
ATOM	2928	9	ARG	641	36.119	49.879	69.655	1.00 19.51 3
ATOM	2929	N	TRP	642	37.972	49.598	68.366	1.00 16.84
ATOM	2930	CA	TRP	642	38.925	49.723	69.515	1.00 14.61 5
ATOM	2931	CB	TRP	642	38.765	48.534	70.453	1.00 13.71 5
ATOM	2932	CG	TRP	642	39.106		63.819	1.00 9.75 5
MOTA	2933		TRP	642	38.203		69.133	1.00 10.16 #
MOTA	2934		TPP	642	38.926		68.814	1.00 10.08 6
ATOM	2935		TP.P	642	36.855		68.760	1.00 8.27 6
ATOM	2936			642	40.304		69.860	1.00 7.42 4
MOTA	2937		TRP	642	40.208		69.267	1.00 10.16 7
MOTA	2938		TRP	642	38.345		68.150	1.00 8.53 ÷
ATOM	2939		TPP	642	36.289		68.098	1.00 7.26 6 1.00 7.13 6
ATOM	2940		TRF	642	37.035		67.803	1.00 T.13 5
MOTA	2941	C	TRF	642	40.424		69.178	1.00 15.14 ÷
ATOM	2942	0	TPP	642	40.798		68.006	1.00 17.51 3
ATOM	2243	N	LEU	643	41.275		70.207	1.00 13.07 -
ATOM	2944	CA	LEU	643	42.747		70.039	1.00 13.34 5
ATOM	2945	CB	LEU	643	43.310		70.676	1.00 9.27 4 1.00 9.05 5
ATOM	2946	CG	LEU	643	42.887		70.081	
ATOM	2947		LEU	643	43.784		70.583	1.00 7.00 5
ATOM	2948		LET	643	43.013		€8.601	1.00 9.98
ATOM ATOM	2949	C	LEU	643	43.508		70.662	1.00 15.42 6
ATOM	2950	0	LEU	643	43.096		71.697	3.00 19.66
ATOM	2951 2952	СD И	PRO	644	44.645		70.059	1.00 15.88
ATOM	2952	CA	PRO	644	45.206		68.817	1.00 15.21 5
ATOM	2954	CB	PRC PRC	644	45.481		70.556	1.00 14.66 3 1.00 15.17 3
ATOM	2955	CG	PRC	644	46.485 46.642		69.412	1.00 15.17
ATOM	2956	C	PRO	644	46.192		68.867	1.00 15.08 E
		_		~77	30.492	4000	71.851	1.00 11.57

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ATOM	2957	o :	PRO	644	46	.148			72.209	1.00 12.33
ATOM	2958		PRO	645		.806			72.588 72.229	1.00 10.67 7
ATOM	2959		PRO	645		.832		.392 .049	73.851	1.00 9.59
MOTA	2960		PRO	645		.530		.746	74.038	1.00 10.22 5
ATOM	2961	CB	PRO	645 645		.321		.742	73.502	1.00 9.51 5
MOTA	2962	CG C	PRO PRO	645		.475		.178	73.572	1.00 9.51
ATOM	2963 2964	0	PRO	645		.211		.142	72.605	1.00 11.71 3
MOTA MOTA	2965	N	PRO	646		3.433		.229	74.375	1.00 9.63 7
ATOM	2966	CD	PRO	646		7.682		.431	75.618	
ATOM	2967	CA	PRO	646		9.334		.350	74.105	1.00 9.90 5
ATOM	2968	CB	PRO	646		9.004		.345	75.217 75.674	1.00 11.92 6
MOTA	2969	CG	PRO	646		7.619 0.809		.956	74.116	1.00 13.01
MOTA	2970	C O	PRC PRO	646 646		1.204		.918	74.679	1.00 14.24 5
MOTA	2971 2972	N	CLU	647		1.620	50	.786	73.470	1.00 13.38 7
atom Atom	2973	CA	GLU	647		3.043		.546	73.383	1.00 14.58 5 1.00 15.62 5
ATOM	2974	CB	GLU	647		3.753		.217	74.552	1.00 15.62 5 1.00 19.18 5
ATOM	2975	CG	GLU	647		3.788		2.737 3.470	74.380 75.640	1.00 20.10 6
ATOM	2976	CD	GLU	647		4.239		3.215	76.715	1.00 22.78
ATOM	2977		GLU	647 647		5.175		4.305	75.563	1.00 19.41 €
MOTA	2978		GLU	647		3.485		9.082	73.218	1.00 14.37
ATOM	2979	0	GLU	647		4.508	4	8.697	73.795	
MOTA	2980 2981	N	THR	648		2.755		8.316	72.384	
ATOM ATOM	2982	CA	THP	64B		53.029		6.899	72.062	
ATOM	2983		THR	648		51.832		5.984	72.452	
ATOM	2984	OGI	THR	648		51.552		6.119	73.852	
MOTA	2985		2 THR	548		52.134		4.533 6.761	72.141 70.534	
MOTA	2986		THR	648		53.295 52.584		7.370	69.715	
MOTA	2987		THR	648 649		54.320		5.968		7 1.00 7.20 7
MOTA	2988		PRO PRO	649		55.333		5.245		1.00 6.54 5
ATOM	2989 2990		PRO	649		54.610		15.819		
MOTA MOTA	2991		PRO	649		56.10		15.495		
ATOM	299	_	PRO	649		56.23		14.592		
ATOM	299		PRO	649		53.82		44.707		
ATOM	299	4 0	PRO	649		52.95		44.106	_	·
MOTA	299		MET	650		54.22 53.64		44.406 43.363		
ATOM	299			650 650		54.15		41.969		0 1.00 8.66 5
ATOM	299			650		55.67		41.83		0 1.00 7.85 🗧
ATOM ATOM	299 299			650		56.21		41.81		
MOTA	300			650		56.57		40.14		
ATOM	300		MET	650		52.11		43.35		· · · · · · · · · · · · · · · · · · ·
ATOM	300	2 0	MET	650		51.47		42.28		
MOTA			THR	651		51.58		44.54		
ATOM				651		49.85		46.19		
ATOM				653 653		50.43		47.19		
ATOM			G1 THR G2 THR			48.3		46.50		87 1.00 15.74 🥱
ATOM ATOM						49.3	53	43.78		
ATOM	-					48.3		43.26		
ATON	-					49.8		43.47		
1OTA			A SEF			49.1 49.5		42.62		
MOTA			B SEF			30.4		41.99		
ATO:			G SEF			49.2		41.1		
ATO! ATO!			SEI			49.0	34	40.2		
ATO		-	J HI			49.5		40.7		
ATO			A HI	5 65		49.5		39.3		
ATO		18 (CB HI			50.9		39.0		
ATO			CG HI			51.8 52.2		38.9 37.8		
ATO			CD2 HI		53	52.4		40.0		
λTO			ND1 HI		53 53	53.1		39.6		
ATO			CE1 HI NE2 HI		53	53.0		38.3		
ATO		_	C HI	-	53	48.4		39.1	63 65.	
ATC ATC			O HI		53	47.	9 B9	38.0		
ATC			N IL		54	48.		40.2		
ATC			CA IL	.E 6	54	47.		40.1		
ATC	M 31		CB II			47.		41.4		355 1.00 3.95 653 1.00 5.93
ATO		029	CG2 II		54 54	46.	252 469	41.5		760 1.00 3.24
ATO		030	CG1 II		54 54		469 560	43.		131 1.00 2.00
ATC		031 032	CD1 II		54		633	39.		156 1.00 5.10
TA TA		033			54	44.	981	40.	508 65.	395 1.00 7.39
AT		034			55	45.	214	38.	661 E7.	713 1.00 5.70

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ATOM	3035	CA	ARG	655	43.856	38.107	67.582	1.00 4.70	á
ATOM	3036	CB	ARG	655	43.947	36.608	67.851	1.00 6.54	6
ATOM	3037	CG	ARG	655	42.732	35.835	67.393	1.00 12.78	5
ATOM	3038	CD	ARG	655	42.923	35.234	66.013	1.00 19.16	é
ATOM	3039	NE	ARG	655	41.690	35.243	65.243	1.00 25.22	7
ATOM	3040	CZ	ARG	655	41.487	34.509	64.155	1.00 28.18	5
ATOM	3041	NH 1		655	42.441	33.699	63.683	1.00 29.93	7
ATOM	3042		ARG	655	40.343	34.523	63.465	1.00 30.11	7
ATOM	3043	Ç	ARG	655	43.012	38.786	68.687	1.00 4.93	6
ATOM	3044	0	ARG	655	43.561	39.225	69.706	1.00 4.78	3
atom atom	3045 3046	N CA	TYR TYR	656 656	41.706 40.852	38.916	68.485	1.00 3.05	7
ATOM	3047	CB	TYR	656	40.315	39.533 40.886	69.491 69.041	1.00 4.57 1.00 5.74	6
ATOM	3048	CG	TYR	656	41.339	41.973	69.131	1.00 5.74 1.00 11.08	6 6
ATOM	3049		TYP	656	41.994	42.423	67.995	1.00 11.86	6
ATOM	3050	CE1		656	43.029	43.341	68.077	1.00 13.79	6
ATOM	3051	CD2	TYR	656	41.736	42.482	70.366	1.00 13.83	6
ATOM	3052	CE2	TYR	656	42.779	43.407	70.461	1.00 14.75	6
ATOM	3053	CZ	TYR	656	43.422	43.826	69.307	1.00 14.26	6
ATOM	3054	OH	TYR	656	44.498	44.701	69.373	1.00 19.33	8
ATOM	3055	С	TYR	656	39.693	38.646	69.848	1.00 7.31	6
ATOM	3056	0	TYP.	656	39.504	37.608	69.210	1.00 7.58	â
ATOM	3057	N	GLU	657	38.967	39.048	70.905	1.00 9.63	7
ATOM ATOM	3058 3059	CA CB	GLU GLU	657 657	37.776	38.359	71.431	1.00 9.06	6
ATOM	3060	CG	GLU	657	38.109 36.874	37.385 36.766	72.555 73.217	1.00 11.39	6
ATOM	3061	CD	GLU	657	36.755	35.254	72.977	1.00 14.76 1.00 17.29	6 6
ATOM	3062	GE1		657	36.157	34.838	71.945	1.00 19.32	8
ATOM	3063		GLU	657	37.245	34.472	73.826	1.00 18.57	8
ATOM	3064	С	GLU	657	36.827	39.366	72.006	1.00 10.04	6
ATOM	3065	0	GLU	657	37.163	40.033	72.985	1.00 8.78	8
ATOM	3066	N	VAL	658	35.635	39.428	71.412	1.00 13.32	7
ATOM	3067	CA	VAL	658	34.550	40.334	71.819	1.00 15.04	6
ATOM	3068	CB	VAL	658	33.826	40.908	70.578	1.00 17.13	6
ATOM	3069		VAL	658	32.355	41.228	70.903	1.00 18.15	6
ATOM	3070		VAL	658	34.552	42.151	70.055	1.00 15.29	6
ATOM ATOM	3071 3072	C	VAL VAL	658 658	33.518	39.602	72.697	1.00 15.57	6
ATOM	3072	N	ASP	65 8 65 9	33.025 33.168	38.519 40.225	72.336	1.00 16.39	8
ATOM	3074	CA	ASP	659	32.217	39.660	73.818 74.762	1.00 15.80 1.00 16.22	7 6
ATOM	3075	СВ	ASP	659	32.857	39.583	76.152	1.00 18.33	6
ATOM	3076	CG	ASP	659	31.841	39.320	77.262	1.00 17.02	6
ATOM	3077	OD1	ASP	659	31.70€	40.220	78.127	1.00 16.96	ā
ATOM	3078	OD2	ASP	659	31.191	38.238	77.248	1.00 15.05	а
ATOM	3079	С	ASP	659	30 .95 9	40.488	74.877	1.00 17.09	6
ATOM	3080	0	ASP	659	30.946	41.480	75.641	1.00 16.55	3
ATOM	3081	N	VAL	660	29.924	40.096	74.127	1.00 17.40	7
ATOM	3082	CA	VAL	660	28.623	40.775	74.150	1.00 18.10	ŕ
atom atom	3083 3084	CB	VAL VAL	660 660	27.835	40.550	72.857	1.00 15.37	5
ATOM	3085		VAL	660	28.760 26.931	40.397 39.368	71.683 72.990	1.00 16.34	5
ATOM	3086	C	VAL	660	27.768	40.299	75.335	1.00 15.04 1.00 20.40	5 5
ATOM	3087	õ	VAL	660	27.719		75.635	1.00 20.40	8
ATOM	3088	N	SER	661	27.018		75.943	1.00 22.33	7
ATOM	3089	CA	SER	661	26.210		77.104	1.00 23.37	6
ATOM	3090	CB	SER	661	27.146		78.308	1.00 23.56	6
ATOM:	3091	OG	SER	661	28.007	39.569	78.169	1.00 25.08	а
MOTA	3092	. с	SER	661	25.132		77.544	1.00 25.29	6
ATOM	3093	9	SER	661	24.814		76.839	1.00 24.57	а
ATOM	3094	N	ALA	662	24.676		78.784	1.00 26.02	7
ATOM	3095	CA	ALA	662	23.690		79.598	1.00 23.48	5
MOTA MOTA	3096 3097	CB C	ALA ALA	662 662	23.909		79.493	1.00 24.66	5
ATOM	3098	õ	ALA	662	22.242 21.935		79.339 79.266	1.00 22.08 1.00 16.69	.5
ATOM	3099	N	GLY	663	21.367		73.300	1.00 23.15	3 7
ATOM	3100	CA	GLY	663	19.936		79.047	1.00 24.87	5
ATOM	3101	C	GLY	663	19.124		80.038	1.00 23.53	5
ATOM	3102	O	GLY	663	18.542		73.649	1.00 22.72	я
MOTA	3103	N	ASN	664	19.032		81.277	1.00 24.09	7
ATOM	3104	CA	ASN	654	18.317		82.410	1.00 25.56	ń
ATOM	3105	CE	ASN	664	17.157		82.938	1.00 27.33	ń
ATOM ATOM	3106	CG	ASN	664	15.907		82.013	1.00 28.05	6
ATOM	3107 3108		ASN ASN	664 664	15.791		81.114	1.00 29.36	3
ATOM	3109	C	ASN ASN	664 664	14.939 17.831		82.294	1.00 26.86	.,
ATOM	3110	Ö	ASN	664	16.97		82.334 81.488	1.00 25.78 1.00 25.92	- 5 - 8
ATOM	3111	N	GLY	665	18.250		83.243	1.00 24.45	9
ATOM	3112	CA	GLY	665	17.91		82.294	1.00 24.29	6
					· -		•		,

bref21	c.pdb		Thu	Apr	25	12:	27:47	1996	41	
ATOM :	3113 0	GLY	665		8.56			82.235	1.00 23.94 5 1.00 24.01 5	
ATOM :	3114 0				8.75		6.011 7.805	82.454 81.047	1.00 22.31	
	3115 N				B.76		7.054	80.035	1.00 22.71	
		A ALA			9.33		7.724	78.693	1.00 21.95	5
		B ALA		-	20.89		7.166	80.577	1.00 24.38	5
		ALA			21.30		8.225	81.075	• • • • • • • • • • • • • • • • • • • •)
		N GLY		:	21.57		6.036	80.672		7 5
ATOM		CA GLY	667		22.94		6.058	81.159		į
ATOM	3122	C GLY			23.83		5.946	79.949 79.937		§
ATOM		o GLY			24.78 23.48		5.145	78.896		7
ATOM		N SE			24.25		6.669	77.641	1.00 28.04	6
ATOM		CA SEI CB SEI			23.63		7.605	76.547		6
ATOM ATOM		OG SEI			24.31		37.574	75.278		8
ATOM		C SE	R 668		25.5		37.209	78.057	1.00 27.60 1.00 27.37	6 8
ATOM	3129	O SE			25.64		38.220 36.397	78. 79 8 77. 76 2	1.00 26.59	7
MOTA	3130	N VA			26.6		36.715	77.987	1.00 23.08	6
MOTA	3131	CA VA			28.6		35.974	79.266	1.00 20.59	6
ATOM	3132 3133	CB VA			28.4		34.484	79.178	1.00 19.42	5
ATOM ATOM	3134	CG2 VA			30.1		36.316	79.456	1.00 20.06	6
ATOM	3135	C VA			28.6		36.266	76.644	1.00 21.55	5 C
ATOM	3136	O VA	L 669		29.8		35.888	76.545	1.00 20.19	8 7
ATOM	3137	N GI			27.8		36.409	75.598	1.00 20.21 1.00 18.75	6
ATOM	313B	CA GI			28.1		36.009 36.236	74.245 73.312	1.00 17.59	6
MOTA	3139	CB GI			27.1		35.569	71.935	1.00 22.13	5
ATOM	3140 3141	CC GI			27.9		36.432	70.902	1.00 22.70	6
MOTA MOTA	3142	OE1 G			28.		37.485	71.234	1.00 24.66	8
ATOM	3143	NE2 G)	27.9		35.995		1.00 23.69	7 6
ATOM	3144		LN 670		29.		36.583 37.782		1.00 17.46 1.00 15.56	8
MOTA	3145		LN 670		29. 30.:		35.679		1.00 15.69	7
ATOM	3146		RG 671 RG 671		31.		36.013		1.00 16.60	6
ATOM	3147 3148		RG 67		32.		35.334			6
ATOM ATOM	3149		RG 67:		32.		36.061			6
ATOM	3150		RG 67		32.		35.269			6
ATOM	3151		RG 67	1	32.		35.894			7 6
MOTA	3152		RG 67			863	35.344			7
MOTA	3153	NH1 A				370 304	34.124 36.062			7
ATOM	3154	NH2 A	RG 67 RG 67			869	35.66			6
atom Atom	3155 3156		RG 67			425	34.61			8
ATOM	3157		AL 67		32.	576	36.55			7
ATOM	3158	CA V	AL 67			879	36.33			6 5
MOTA	3159		AL 67			.079	37.31 37.44			š
MOTA	3160	CG1 V				. 649 . 728	38.70			6
ATOM	3161	CG2 1	7AL 67 7AL 67			379	36.53			6
MOTA MOTA	3162 3163		VAL 67			. 964	37.49			8
ATOM	3164			13		.011	35.58			?
ATOM	3165	CA		13	36	.437	35.66			6 5
MOTA	3166		-	73 73		. 902 . 621	34.40			5
ATOM	3167			73 73		. 996	33.29			÷
MOTA MOTA	3168 3169			73		. 964	32.15			9
ATOM		· OE2		73		.279				3
ATOM			GLU 6	73		. 645				რ 9
MOTA	3172	2 ¢	_	73		. 688				7
MOTA				74		1.899 3.224				Ę
ATOM			-	74 74		3.340				÷
ATOM ATOM				74		3.785				÷
ATOM				74		7.060		44 67.2		5
ATOM				74		5.824				
ATOM		9 C		574		9.596				5 3
ATOM	318			574		0.511				
ATOM			-	675 575		9.722 1.000				
ATON				675 6 7 5		0.B4				
MOTA MOTA				675		0.33		55 61.3	59 1.00 17.94	. 5
ATO				675	3	8.78	6 36.0			
ATO	4 318	6 CD2	LEU	675		0.96				
ATO				675 675		1.94				
ATO:				675 676		1.50				
OTA			GLU	676		4.31				

bref2	21c.p	đb		Thu	Apr 25	12:27:47	1996		42	
MOTA	3191	СВ	GLU	676	45.667	38.907	63.526	1.00	12.08	ŧ
ATOM	3192	CG	GLU	676	45.627		62.478		11.18	
ATOM	3193	CD	GLU	676	45.494		63.080	1.00	13.77	÷
ATOM ATOM	3194 3195	OE1	GLU	676 676	46.538		63.546		16.32	=
ATOM	3196	C	GLU	676	44.367 44.268		63.108 63.146		13.00	=
ATOM	3197	0	GLU	676	43.569		62.159		12.13 12.89	•
ATOM	3198	N	GLY	677	45.030	41.772	63.699		11.52	3
ATOM	3199	CA	GLY	677	45.121		63.145		11.07	:
ATOM ATOM	3200	C	GLY	677	43.796		62.961		11.96	=
ATOM	3201 3202	O N	GLY ARG	677 678	43.770 42.700		62.523		14.32	=
ATOM	3203	CA	ARG	678	41.387		63.329 63.174		12.98	
ATOM	3204	CB	ARG	678	40.342		62.927		13.34	÷
ATOM	3205	CG	ARG	678	39.529		61.695		15.05	į
MOTA	3206	CD	ARG	678	40.401		60.504		17.70	- 5
atom Atom	3207 3208	NE CZ	ARG ARG	678 678	41.014 41.887		60.643		22.61	
ATOM	3209		ARG	678	42.274		59.787 58.700		23.28	€ 1:
MOTA	3210		ARG	678	42.380		60.037		22.06 25.26	_
ATOM	3211	С	ARG	678	41.001	44.532	64.420		14.43	£
ATOM ATOM	3212	0	ARG	678	41.199		65.529	1.00	15.07	3
ATOM	3213 3214	N CA	THR	679 679	40.462		64.249		13.15	
ATOM	3215	CB	THP	679	40.027 40.996		65.390		14.13	÷
ATOM	3216	OG1		679	41.204		65.669 64.448		14.19 17.57	•
ATOM	3217	CG2		679	42.332		66.229		13.59	•
ATOM	3218	С	THP	679	38.637		65.182		16.43	
ATOM	3219	0	THP	679	38.393		65.540		15.23	
ATOM	3220	N	SLU	680	37.732		64.604		18.09	-
ATOM ATOM	3221 3222	CA CB	GLU GLU	680 680	36.358		64.332		19.04	£
ATOM	3223	CG	GLU	680	36.289 36.140		63.128		18.69	•
ATOM	3224	CD	GLU	680	35.086		61.755 60.847		18.32	ē
ATOM	3225		GLU	680	34.342		60.138		16.53	3
ATOM	3226		GLU	680	35.019		60.825		14.40	3
ATOM	3227	Ç	GLU	680	35.489		64.076	1.00	21.29	5
ATOM ATOM	3228 3229	0	CIS	680 681	35.887 34.299		63.364		22.54	3
ATOM	3230	CA	CYS	681	33.382		64.654 64.498		22.91	
ATOM	3231	CB	CYS	681	33.617		65.603		24.61 26.42	÷
ATOM	3232	SG	CYS	681	32.134		66.606		26.71	<u>.</u> .
ATOM	3233	С	23.2	681	31.958		64.540		24.30	:
ATOM ATOM	3234 3235	O N	CYS	681	31.579		65.448		23.84	-
ATOM	3236	CA	7AL	682 682	31.181 29.818		63.517		21.58	
ATOM	3237	CB	VAL	682	29.433		63.511		20.10	£
ATOM	3238	CG1	VAL	682	30.190		60.969		16.40	Ē
ATOM	3239		VAL	682	27.952	45.785	61.867		17.19	É
ATOM	3240	C	7AL	682	28.861		64.001		17.00	÷
atom Atom	3241 3242	O N	VAL LEU	682	28.659		63.342		15.10	Ē
ATOM	3242	CA	LEU	683 683	28.449 27.485		65.258		17.47	
ATOM	3244	CB	EE	683	27.326		65.859		20.70	:
ATOM	3245	CG	LEU	683	28.420		68.299		17.50 13.82	:
ATOM	3246	CD1	LET	683	28.201		69.667		13.45	:
ATOM	3247		LEU	683	28.376		68.387		15.36	:
atom atom	3248 3249		LEU	683	26.228		65.104		24.03	: :
ATOM	3250	Ŋ	SER	683 684	25.446 26.087		65.544		24.27	-
ATOM	3251	CA	SER.	684	25.003		63.914 63.028		25.99 26.98	:
ATOM	3252	CB	SEF.	684	25.222		61.629		31.20	:
ATOM	3253	OG	SEP.	684	26.502		61.067		36.99	
MOTA	3254	c	SER	684	23.614		63.491	1.00	26.69	:
ATOM ATOM	3255 3256	O N	IER.	584 685	22.800		63.699		27.76	:
ATOM	3257	CA	ASN ASN	685 685	23.397 22.049		63.826		24.94	-
ATOM	3258	CB	ASX	685	21.716		64.131 63.083		25.85	:
ATOM	3259	CG	AEN	685	22.993		62.504		27.66 28.61	
ATOM	3260		AE::	685	23.994	40.433	62.186		26.41	÷
ATOM	3261		ZEA	685	22.972	38.406	62.407	1.00	28.57	-
MOTA MOTA	3262 3263	Ō.	ASN ASN	685 685	21.748		65.533		26.76	3
ATOM	3264	N	LEU	685 686	22.271 20.899		€5.923		27.14	:
ATOM	3265	CA.	LE:	686	20.583		66.287 67. 64 9		25.95 24.26	
ATOM	3266	CB	LEU	686	21.779		68.584		22.44	:
ATOM	3267	CG	LEC	686	22.718	42.760	68.474		23.47	
ATOM	3268	CDI	LEU	686	23.700	42.840	69.708		21.84	- ;

bref21	.c.pd	b		Thu	Apr	25	12:	27:4	47	1996		43		
ATOM	3269	CD2	LEU	686		3.5		42.74		7.173	1.00 2		5 5	
MOTA	3270	C	LEU	686		9.23		41.56 40.66		8.478	1.00		3	
MOTA	3271 3272	0	LEU ARG	686 687		9.0		42.80		8.858	1.00		7	
ATOM ATOM	3273	CA	ARG	687		7.8		43.14		9.636	1.00		5	
ATOM	3274	CB	ARG	687		8.1		42.90		71.113 71.745	1.00		5	
ATOM	3275	CG	ARG	687		17.2		41.84 40.47	_	71.410	1.00		5	
ATOM	3276	CD	ARG ARG	687 687		16.8		39.42		71.911	1.00	23.57		
ATOM ATOM	3277 3278	NE CZ	ARG	687		16.8		38.18	8	71.416		24.78		
MOTA	3279	NH1		687		17.6		37.83		70.405	-	25.89 23.14		
ATOM	3280	NH2	ARG	687		15.9		37.30		71.908 69.517		23.14		
MOTA	3281	C	ARG	687		17. 3 17.8		44.58		68.695		24.06		
ATOM	3282	0 N	ARG GLY	687 688		16.4		44.93		70.407		23.79	, -	
ATOM ATOM	3283 3284	CA	GLY	688		15.8		46.26		70.434		22.75		5
ATOM	3285	С	GLY	688		15.5		46.64		71.874		23.19		6 B
ATOM	3286	0	GLY	688		15.3		45.70		72.726 72.154		23.01		7
ATOM	3287	N	ARG ARG	689 689		15.3		48.5		73.500		23.70		6
ATOM	3288 3289	CB	ARG	689		14.0		48.5		73.902		22.8		6
MOTA MOTA	3290	CG	ARG	689		13.	543	49.8		74.581		20.4		6
ATOM	3291	CD	ARG	689		13.		50.9		73.575		18.4		6 7
MOTA	3292	NE	ARG	689		14.		52.2 52.8		73.908 75.128		19.2		5
MOTA	3293	CZ	ARG	689		14.		52.2		76.250		12.8		7
ATOM	3294 3295		ARG ARG	689 689		14.		54.0		75.213	1.00	18.7	1	7
MOTA MOTA	3296	C	ARG	689		16.		47.9		74.648		25.8		á
ATOM	3297	0	ARG	689			512	48.5		75.756		25.2 25.7		8 7
ATOM	3298		THR	690			153 053	46.8		74.313 75.182		23.9		6
ATOM	3299			690 690			530	44.9		74.403		24.9		6
ATOM ATOM	3300 3301		1 THP.	690			550	44.5		73.405		24.9		8
ATOM	3302		2 THR	690			808	43.		75.355		24.3		ა 6
MOTA	3303		THR	690			337	46.8		75.661 74.841		27.3 25.8		8
ATOM	3304		THR	690			052	47.4		76.966		28.0		ž
MOTA	3305		ARG	691 691			653 920	47.		77.514		27.		6
ATOM	330 <i>6</i> 3301						908	47.		79.055		28.	38	6
ATOM ATOM	3308						. 668	46.		79.860		30.		5 5
ATOM	3309	e cr					.736	46.		81.403 82.240		0 30. 0 29.		7
MOTA	3310						.360 .681		549 632	82.95		0 31.		5
ATOM	331: 331:		Z ARG				.331		612	82.93	1.0	0 32.		7
MOTA ATOM	331		12 ARC				.337	_	775	83.76		0 28.		7 5
ATOM	331		ARC				.024		269	77.11		0 27. 0 28.		8
MOTA	331		ARC				.863		781	76.68		0 27.		7
MOTA	331 331						.213		B93	76.25		0 23.		5
MOTA MOTA	331						.237		. 885	74.74		0 24.		5
ATOM	331						.317		905	74.10		0 23.		5 5
ATOM	332		D1 TY				.303		. 5 75			00 23. 00 23.		6
MOTA			El TY				2.544	5 45	. 6 36 . 28 3			0 24.	04	5
ATOM ATOM			D2 TY				.75		. 345		5 1.0	00 24	. 91	6
ATOM			Z TY			2:	1.77	2 43	.022			00 24		5
ATOM		25 0	H TY	R 69			1.02		.086			00 27. 00 22		8 6
ATOM							5.53 5.77		.436			00 21		8
ATOM			TY TH				6.3B		.567			00 19		7
ATOM ATOM			CA TH			2	7.71	1 45	. 989	77.7	8 1.	00 14		ó
ATOM		-	св ТЕ	IR 69			7.87		. 985			00 13		ร์ 8
ATOM	1 33		OG1 TH				6.74		. 642			00 14 00 12		ń
ATON		_	CG2 TH		93 93		9.15 8.70		5.74			00 14		- 6
1OTA 1OTA		-	C TH O TH				B.45		.87			00 11		8
ATO			N PI	HE 6	94	2	9.81	.1 4	5.66			00 15		7
ATO	M 33	36			94		0.84		1.96			00 15		ő
ATO					94		9.4	_	5.50 5.68			00 19		Ģ
ATO		38	CG P		94 94		B.74		6.86			00 18		6
ATO:		40	CD2 P		94		8.0	32 4	4.67	9 73.0	15 1.	.00 18	3.42	6
ATO		41	CE1 P	HE 6	94		27.41		7.03			.00 1		- i
ATO	M 33	42	CE2 P		94		27.6		4.85 6.02			.00 1		6 6
ATO		343			94 94		26.9: 32.2		5.21			.00 1		
ATC ATC		344 345			94		32.5		6.30			.00 1		3
ATC		346			595		33.1		4.22		.55 1	.00 1	4.22	••

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ATOM	3347	CA	ALA	695	34.532	44.271	76.533	1.00 14.58 6
ATOM	3348	CB	ALA	695	34.704	43.821	77.959	1.00 14.58 6 1.00 15.52 6
ATOM	3349	С	ALA	695	35.331	43.352	75.579	1.00 16.59 6
ATOM	3350	0	ALA	695	34.739	42.503	74.883	1.00 16.77 6
ATOM	3351	N	VAL	696	36.663	43.475	75.554	1.00 18.89 7
ATOM	3352	CA	VAL	696	37.475	42.637	74.640	1.00 18.54 6
MOTA MOTA	3353 3354	CB CG1	VAL VAL	696 696	37.455 37.867	43.242	73.198	1.00 19.19 6
ATOM	3355		VAL	696	38.335	44.705 42.446	73.223	1.00 17.15 6
ATOM	3356	c	VAL	696	38.923	42.284	72.255 75.047	1.00 20.60 6 1.00 18.64 6
ATOM	3357	0	VAL	696	39.654	43.093	75.637	1.00 18.64 6 1.00 18.43 8
ATOM	3358	N	ARG	697	39.321	41.055	74.738	1.00 18.97 7
ATOM	3359	CA	ARG	697	40.675	40.563	75.050	1.00 18.67 6
ATOM	3360	CB	ARG	697	40.593	39.173	75.664	1.00 17.03 6
ATOM	3361	CG	ARG	697	39.772	39.078	76.889	1.00 15.40 6
ATOM ATOM	3362 3363	CD NE	ARG ARG	697 69 7	39.842 39.077	37.650	77.417	1.00 18.07 6
ATOM	3364	CZ	ARG	697	38.722	36.676 35.467	76.632 77.081	1.00 17.47 7
ATOM	3365	NH1	ARG	697	39.061	35.078	78.309	1.00 19.24 6 1.00 20.70 7
ATOM	3366		ARG	697	38.014	34.643	76.318	1.00 18.93 7
MOTA	3367	C	ARG	697	41.625	40.494	73.818	1.00 18.98 6
MOTA	3368	0	ARG	697	41.180	40.255	72.677	1.00 19.20 8
MOTA	3369	N	ALA	698	42.926	40.660	74.077	1.00 17.10 7
ATOM	3370	CA	ALA	698	43.973	40.609	73.057	1.00 14.99 6
ATOM ATOM	3371 3372	CB	ALA	698	44.816	41.858	73.146	1.00 15.98 6
ATOM	3373	CO	ALA ALA	698 698	44.838 45.073	39.366	73.296	1.00 14.49 6
ATOM	3374	N	ARG	699	45.349	38.999 38.753	74.432	1.00 16.90 8
ATOM	3375	CA	ARG	699	46.174	37.540	72.325	1.00 13.57 7 1.00 10.72 6
ATOM	3376	CB	ARG	699	45.229	36.331	72.392	1.00 12.04 6
MOTA	3377	CG	ARG	699	45.692	35.014	71.794	1.00 12.63 6
ATOM	3378	CD	ARG	699	46.738	34.349	72.665	1.00 20.39 6
ATOM	3379	NE	ARG	699	46.913	32.910	72.399	1.00 21.37 7
atom Atom	3380 3381	CZ	ARG ARG	699	46.119	31.955	72.895	1.00 21.92 6
ATOM	3382	NH2	ARG	699 699	45.069 46.442	32.257 30.682	73.672	1.00 21.47 7
ATOM	3383	C	ARG	699	47.090	37.470	72.710 71. 094	1.00 22.33 7 1.00 9.38 6
MOTA	3384	ō	ARG	699	46.680	37.820	69.991	1.00 9.38 6 1.00 10.86 8
ATOM	3385	N	MET	700	48.355	37.109	71.282	1.00 8.21 7
ATOM	3386	CA	MET	700	49.263	37.029	70.140	1.00 7.21 6
ATOM	3387	CB	MET	700	50.724	36.955	70.551	1.00 6.01 6
ATOM	3388	CG	MET	700	51.322	38.292	70.963	1.00 5.33 6
ATOM	3389	SD	MET	700	52.092	39.250	69.678	1.00 9.84 16
ATOM ATOM	3390 3391	CE	MET MET	700 700	51.368 48.875	40.792	69.955	1.00 8.49 5
ATOM	3392	ō	MET	700	48.609	35.808 34.755	69.375 69.939	1.00 6.64 6
ATOM	3393	N	ALA	701	48.849	35.943	68.069	1.00 6.32 8 1.00 7.50 7
ATOM	3394	CA	ALA	701	48.425	34.837	67.250	1.00 8.94 6
MOTA	3395	CB	ALA	701	47.605	35.361	66.065	1.00 7.41 6
ATOM	3396	С	ALA	701	49.483	33.855	66.779	1.00 9.12 6
ATOM	3397	0	ALA	701	50.679	34.165	66.639	1.00 9.86 3
MOTA MOTA	3398 3399	N	GLU	702	48.980	32.669	66.491	1.00 10.01 7
ATOM	3400	CA CB	GLU	702 702	49.763	31.574 30.275	65.987	1.00 13.16 6
MOTA	3401	CG	GLU	702	48.724	29.784	66.108 67.501	1.00 15.92 6 1.00 18.17 6
MOTA	3402	CD	GLU	702	48.597	28.284	67.507	1.00 18.17 6 1.00 21.01 5
MOTA	3403	OE1	GLU	702	47.904	27.731	66.611	1.00 22.10 8
MOTA	3404	. 0E2		702	49.233	27.652	68.377	1.00 24.81 8
ATOM	3405	С	GLU	702	50.126		64.510	1.00 13.07 6
ATOM	3406	0	GLU	702	49.560	32.617	63.802	1.00 12.10 8
atom atom	3407 3408	И	PRO	703	51.106	30.986	64.037	1.00 14.95
ATOM	3409	CD CA	PRO PRO	703 703	51.501 51.783	30.820	62.625	1.00 17.31 6
ATOM	3410	CB	PRC	703	51.896	30.007 28.794	64.899	1.00 14.84 5
ATOM	3411	CG	PRO	703	52.253	29.467	63.999 62.635	1.00 14.77 5 1.00 19.35 6
ATOM	3412	c	PRO	703	53.150		65.409	1.00 19.35 6 1.00 13.50 6
ATOM	3413	0	PRC	703	53.801		66.157	1.00 15.09 9
ATOM	3414	N	SER	704	53.587	31.681	65.002	1.00 11.82
ATOM	3415	CA	SER	704	54.873		65.461	1.00 9.78 5
ATOM ATOM	3416	CP CC	SER	704	55.156		64.798	1.00 9.23 6
ATOM	3417 3418	င ၁၆	SER SER	704 704	55.301	33.474	63.394	1.00 E.65 H
ATOM	3419	Ö	SER	704	54.860 55.621		67.003 67.736	1.00 11.09 5
ATOM	3420	N	PHE	705	53.937		67.468	1.00 12.01 A 1.00 8.75 7
ATOM	3421	CA	PHE	705	53.767		68.857	1.00 3.52 6
ATOM	3422	CB	PHE	705	53.323	34.973	68.988	1.00 5.09 6
MOTA	3423	CC	PHE	705	54.159		68.184	1.00 7.49 6
ATOM	3424	CUI	PHE	705	53.696	36.417	66.957	1.00 8.92 6

bref21	lc.pdl	b		Thu	Apr	25	12	: 27 : 47	19	96		45	
ATOM	3425	CD2	PHE	705		55.4		36.284	68.		1.00	8.54	: :
ATOM	3426	CEL		705		54.5		37.252	66.		1.00	7.44 4.91	e e
MOTA	3427		PHE	705		56.2 55.8		37.115 37.598		833 606	1.00	5.19	á
MOTA	3428	CZ	PHE	705 705		52.7		32.591		505	1.00	5.11	÷
MOTA	3429	C	PHE PHE	705		52.2		31.697		878	1.00	4.57	3
ATOM	3430 3431	O N	GLY	706		52.6		32.751	70.	809	1.00	8.69	7
MOTA MOTA	3432	CA	GLY	706		51.7		31.956		622	1.00	7.99	÷
ATOM	3433	ς	GLY	706		51.€	61	32.726		932	1.00	9.39	e ÷
ATOM	3434	0	GLY	706		52.3		33.739		.069	1.00	9.05	7
ATOM	3435	N	GLY	707		50.8		32.295		878	1.00	10.91 9.87	5
ATOM	3436	CA	GLY	707		50.		32.990		.162 .977	1.00	7.80	5
MOTA	3437	C	GLY	707		49.4		32.823		.063	1.00	7.37	3
ATOM	3438	0	GLY	707 708		48.		33.927		.540	1.00	7.59	7
MOTA	3439 3440	N CA	PHE	708		47.1		33.911	_	.372	1.00	8.42	5
atom Atom	3441	CB	PHE	708		48.		33.981		.874	1.00	9.14	5
MOTA	3442	CG	PHE	708		49.		33.126		.277	1.00	8.19	ę
ATOM	3443	CD1	PHE	708		49.		31.787		.592	1.00	5.98 6.32	÷
MOTA	3444		PHE	708		50.		33.679		.352	1.00	8.74	5
MOTA	3445		PHE	708		50. 51.		31.016		.731	1.00	5.05	é
ATOM	3446		2 PHE	708 708			570	31.587		.040	1.00	4.00	grant on P
ATOM	3447	cz	PHE PHE	708			846	35.066		.077	1.00	7.99	ē
ATOM	3448 3449	CO	PHE	708			260	36.187		.721	1.00		\$
ATOM ATOM	3450	N	TPP	709			562	34.777		.285	1.00		7
ATOM	3451	CA	TRP	709		44.	475	35.752	_	1.119		12.14	Ę
ATOM	3452	CB	TRP	709			114	35.083		7.396		11.59	\$ \$
ATOM	3453	CG					417	34.592		5.165	1.00	12.07	5
ATOM	3454		2 TRP				098	35.354 34.48		1.999 1.092	1.00		÷
MOTA	3455		2 TRP				. 465 . 283	36.68	_	4.634	1.00		
MOTA	3456		3 TRP				971	33.32		5.929	1.00		_
MOTA	3457		1 TRF				.398	33.25		4.688	1.00	12.13	
MOTA	3458 3459						.018	34.89		2.841	1.00	9.03	
MOTA MOTA	3460						. 838	37.10		3.399		11.59	
ATOM	3461		12 TRE			41	.214			2.513		10.54	
ATOM	3462		TRI	70	9		. 635			8.056			
ATOM	3463		TRI				.770			9.268		0 12.13 0 11.52	
ATOM	3464		SE				.620			7.508 8.351		0 12.14	
ATOM	346						.040			7.501			
ATOM	3460 346						. B47			7.15		0 10.05	5 3
ATOM ATOM	346		SE				.522			9.21		0 12.22	2 5
ATOM	346					42	. 531			9.13		0 17.10	
ATOM	347				1		.580			30.07		0 12.0	1 7
ATOM	347		A AL	A 71	i		. 43			30.89		0 12.4	
MOTA	347	2 C					2.85	_		31.99		0 12.9	
ATOM							1.43			79.96 78.91		0 14.9	_
ATOM							1.810 0.15	_		80.32		0 13.8	
ATOM			TF A TF				9.15			79.52		0 12.5	
ATOM ATOM		-	B TF		2		7.75		31	80.09	2 1.0		
ATOM	_		G T		12	3	7.20	2 40.6		79.84			
ATOM			D2 TI		12		6.79			78.57			
ATOM			E2 T1		12		6.41			78.80 77.27			
ATON		-	E3 T		12		6.71 7.03			80.76			9 5
4OTA			CD1 T		12 12		6.57			80.15			70 7
iota Iota			NE1 T		12		5.96			77.78			16 -
ATO			C23 T		12		6.27		776	76.26	52 1.	00 7.5	
ATO			CH2 T		12	3	5.90			76.52		00 9.0) C =
ATO					12		9.49			79.5		30 12.	
ATO		88			12		10.12			80.4		00 12.	
ATO				_	13		9.1			78.3		30 15.	
ATO					113		39.30			78.1 76.6		00 14.	
ATO					13 113		39.29 37.9			76.1	49	30 11.	50 ∻ 86 ∋
ATO					713		38.1			78.7	99	00 15.	68
ATO ATO		93 94			113		37.0		908	78.7	64 1.	.30 18.	64
ATO		95			714		38.3		705	79.2	79 1.	.00 17.	04
ATO		96			714		37.1		391	79.8		.00 20.	
ATC		197			714		37.5		809	ευ.2		.55 21.	
ATC	M 34	198	CG C	SLU	714		38.4		836	81.4		.00 24.	
ATC		199			714		38.6		179	81.9 82.4		.00 25.	
ATC		500	OE1		714		39.8		.479	82.4 81.9		.00 27.	
ATO		501	OE2		714 714		35.8		.366	79.0		.00 21.	
ATO	,,, 3;	502	C	-			,,,,				-		

bref2	lc.pd	b		Thu	Apr	25	12	:27:47	1996		46	
ATOM	3503	0	GLU	714	3	5.86	7	48.844	77.886	1.00 2	1.24	а
ATOM	3504	N	PRO	715	3	4.78	7	47.852	79.611	1.00 2		7
ATOM	3505	CD	PRO	715	3	4.70	3	47.767	81.090	1.00 2		5
ATOM	3506	CA	PRO	715	3	3.46	0	47.694	79.015	1.00 1		ร์
ATOM	3507	CB	PRO	715	3	2.62	7	47.183	80.182	1.00 2		5
ATOM	3508	CG	PRO	715		3.22		47.974	81.352	1.00 1		5
ATOM	3509	С	PRO	715	3	2.87	4	48.959	78.473	1.00 2		5
ATOM	3510	0	PRO	715	3	3.19	4	50.060	78.922	1.00 2		á
ATOM	3511	N	VAL	716	3	1.93	4	48.769	77.562	1.00 2		7
ATOM	3512	CA	VAL	716	3	1.22	9	49.858	76.910	1.00 1		5
ATOM	3513	CB	VAL	716	3	1.76	9	50.100	75.440	1.00 1		5
ATOM	3514	CG1	VAL	716	3	0.98	8	49.293	74.396	1.00 1		5
ATOM	3515	CG2	VAL	716	3	1.74	9	51.563	75.099	1.00 1		ó
ATOM	3516	С	VAL	716	2	9.77	8	49.366	76.90B	1.00 2		5
ATOM	3517	0	VAL	716	2	9.51	.5	48.182	76.624	1.00 2		ā
ATOM	3518	N	SER	717	2	8.85	9	50.269	77.264	1.00 2		7
ATOM	3519	CA	SER	717	2	7.43	9	49.971	77.331	1.00 2		6
ATOM	3520	CB	SER	717	2	6.92	0	50.181	78.764	1.00 2		5
ATOM	3521	OG	SER	717	2	7.18	2	49.064	79.607	1.00 2	24.17	a
ATOM	3522	С	SER	717	2	6.55	2	50.748	76.375	1.00 2		6
ATOM	3523	0	SER	717	2	6.54	1	51.970	76.394	1.00 1		ā
ATOM	3524	N	LEU	718		5.83		50.014	75.523	1.00 2		7
ATOM	3525	CA	LEU	718	2	4.86	6	50.583	74.585	1.00 2	21.71	5
ATOM	3526	CB	LEU	718		5.00		49.949	73.188	1.00 1	7.72	5
ATOM	3527	CG	LEU	718		4.50		50.860	72.057	1.00 1	5.29	6
ATOM	3528		LEU	718	2	5.27	1	52.197	72.069	1.00]	1.08	6
ATOM	3529	CD2		718		4.63		50.165	70.733	1.00 1	1.73	5
ATOM	3530	С	LEU	718		3.47		50.236	75.183	1.00 2	22.58	5
ATOM	3531	0	LEU	718		3.39		49.506	76.191	1.00 2	24.55	8
ATOM	3532	N	LEU	719		2.39		50.723	74.564	1.00 2		7
ATOM	3533	CA	LEU	719		1.02		50.470	75.054	1.00 2		5
ATOM	3534	CB	LEU	719		0.63		51.586	76.069	1.00 2		6
ATOM	3535	CG	LEU	719		1.54		51.746	77.325	1.00		5
ATOM	3536		LEU	719		1.29		53.039	78.084	1.00 1		5
ATOM	3537		LEU	719		1.41		50.545	78.254	1.00 2		6
ATOM	3538	C	LEU	719		9.98		50.393	73.904	1.00		6
ATOM	3539	0	LEU	719		8.88		50.958	74.036	1.00 2		8
MOTA	3540	N	THR	720		0.32		49.657	72.828	1.00 2		7
ATOM	3541	CA	THP.	720		9.49		49.515	71.597	1.00		6
ATOM	3542	CB	THR	720		9.03		48.042	71.295	1.00		6
ATOM	3543	0G1		720		B.79		47.332	72.513	1.00		8
ATOM	3544	CG2		720		20.04		47.288	70.444	1.00		5
MOTA	3545	C	THP.	720		8.26		50.417	71.492	1.00		5
MOTA	3546	0	THE	720	1	.7.14	• 0	49.947	71.240	1.00 2	22.69	a

Table 1										•	1
Data Set	Resolution	Reflections	Completeness	Rsym	Sites R _{iso} t	R _{iso} †	R _{cullis}	RKraut	Phasing Power	Powers	
	(Å)	(#) 14158	0.93(0.91)	0.05	1	ı	•	1	ı	•	
HgAc ₂	25.0-3.0	11496	0.93 (0.91)	0.10	7	0.102	0.56	0.114	Iso 1.87 (3.1Å) Ano 1.35 (4.0Å)	(3.1Å) (4.0Å)	
UO ₂ (NO ₃) ₂	25.0-3.0	11931	0.96 (0.94)	0.14	4	0.116	0.62	0.137	Iso 1.95 (3.1Å) Ano 1.72 (3.9Å)	(3.1Å) (3.9Å)	,
				RMS fr	om 1de	RMS from ideal values	85	Average	Average B Value (Å ²)	(A ²)	
Refinement	Refinement Statistics:						1			•	
Resolution	Relflections	Relflections Total Number R-value F>10	R-value	Bond Length	ıgth	Bond Angle	Ingle	EBP1	E8P2	repuldes	ı
(c)											
8 C-0 8	13894	3462	0.21		0.0	0.016(Å)	2.1°	10.5	10.5 12.3	10.7	- 1
0.0											

 $*R_{sym}=L|I-<I|/L|I$.

tRiso= El FpH-Fp / LFp.

 $^{\dagger}R_{Cullis}$ = Σ | $F_{
m PH}$ $^{\pm}F_{
m p}|$ $^{-}F_{
m H(calc)}|$ $/F_{
m pH}$ $^{-}F_{
m p}|$ for all centric reflections.

SPhase Power={[] FpH(calc) | 2/2| FpH(obs) Fp(calc) | 1 FpH(obs) Fp(calc) is the lack of closure error to maximum resolution indicated. TR KKRAUT = El FPH(cbs) - FPH(cbs) - FPH(catc) | / E(FPH(cbs) + FPH(cbs) for all acentric relfections (anamalous case).

 4 Completeness of data in the outer shell, (2.9-2.8Å) for the native and (3.1-3.0Å) for both derivatives. Hean Figure of Merit=<| $P(\alpha)e^{i\alpha}/LP(\alpha)|$ > where $P(\alpha)$ is the phase probability.

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Peptidel-EBP1	Peptidel-EBP2	Peptidel-EBP2	Peptide2-EBP1	Peptide2-EBP1 Peptide1-Peptide2	
		;	;		
Gly ^{P9} O-Met ¹⁵⁰ N	Tyr ^{P4} OH-Ser ⁹² N	Gly ^{P9} O-Met ¹⁵⁰ N	Tyr ^{P4} OH-Ser ⁹² N Tyr ^{P4} O-Cys ^{P6} N	TyrP40-CysP6N	
Pro ^{P10} 0-Thr ¹⁵¹ N		Pro ^{P10} 0-Thr ¹⁵¹ N		Tyr ^{P4} N-Cys ^{P6} O	
Pro ^{P10} 0-Thr ¹⁵¹ 0γ		Pro ^{P10} 0-Thr ¹⁵¹ 0γ1		Cys ^{P6} 0-Tyr ^{P4} N	
Leu ^{P11} 0-Ser ¹⁵² N		Leu ^{P11} 0-Ser ¹⁵² N		Cys ^{P6} N−Tyr ^{P4} O	
Leu ^{P11} 0-Ser ¹⁵² 07		Leu ^{P11} 0-Ser ¹⁵² 07			

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CLAIMS

What is claimed is:

- 1. A computer-assisted method for identifying potential mimetics of erythropoietin, using a programmed computer comprising a processor, a data storage system, an input device, and an output device, comprising the steps of:
 - (a) inputting into the programmed computer through said input device data comprising the three-dimensional coordinates of a subset of the atoms in the peptide GGTYSCHFGPLTWVCKPQGG when said peptide is co-crystallized with a portion of the erythropoietin receptor comprising amino acids 1 to 225 of said receptor, thereby generating a criteria data set;
 - (b) comparing, using said processor, said criteria data set to a computer database of chemical structures stored in said computer data storage system;
 - (c) selecting from said database, using computer methods, chemical structures having a portion that is structurally similar to said criteria data set;
- (d) outputting to said output device the selected chemical structures having a portion similar to said criteria data set.

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- 2. A computer-assisted method for identifying potential mimetics of erythropoietin, using a programmed computer comprising a processor, a data storage system, an input device, and an output device, comprising the steps of:
 - (a) inputting into the programmed computer through said input device data comprising the three-dimensional coordinates of a subset of the atoms in the peptide GGTYSCHFGPLTWVCKPQGG when said peptide is cocrystallized with a portion of the erythropoietin receptor comprising amino acids 1 to 225 of said receptor, thereby generating a criteria data set;
 - (b) constructing, using computer methods, a model of a chemical structure having a portion that is structurally similar to said criteria data set;
 - (c) outputting to said output device the constructed model.
- 3. A compound having a chemical structure selected using the method of claim 1, said compound being an EPO mimetic.
 - 4. The compound of claim 3 wherein said compound is not a peptide.
 - 5. The compound of claim 3 wherein said compound is a peptide.
 - 6. The compound of claims 5 wherein said peptide has 15 of fewer amino acids.

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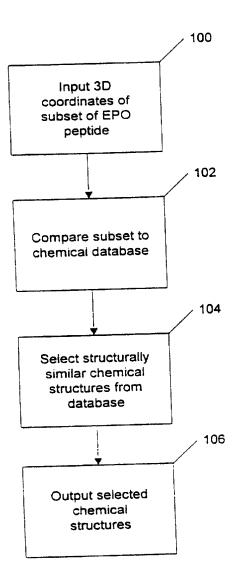


FIG. 1

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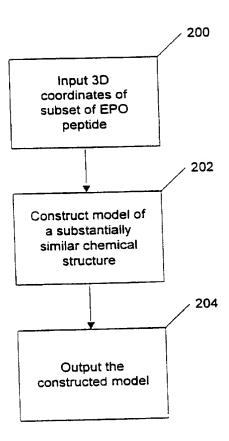


FIG. 2

INTERNATIONAL SEARCH REPORT

International application No. PCT/US97/07218

	SIFICATION OF SUBJECT MATTER		
TIC CI 12	G06F 159:00 364/496]
According to	International Patent Classification (IPC) or to both na	tional classification and IPC	
B. FIEL	DS SEARCHED		
Minimum do	cumentation searched (classification system followed b	y classification symbols)	
	64/496, 497,498,578		!
	on searched other than minimum documentation to the e	extent that such documents are included	in the fields searched
Documentati	on searched other than minimum documentation to the c	Acom distribution de Comment	
Wlastronia de	ata base consulted during the international search (nam	ne of data base and, where practicable,	search terms used)
aps, dialo search te	og Irms: erythropoietin, receptor, 3d, pdb or databa	se	
			
c. Doc	UMENTS CONSIDERED TO BE RELEVANT		
Category*	Citation of document, with indication, where app	ropriate, of the relevant passages	Relevant to claim No.
V	US, 5,331,573 A (BALAJI et al.) 19	a July 1994, (col. 7, lines	1-6
X	46-66, col. 13, lines 20-55, col. 14	4, lines 12-23	
	46-66, Col. 13, lines 25-66, 651.		
A,P	US 5,557,535 A (SRINIVASAN et	al.) 17 September 1996,	1,2
	(abstract, fig. 1, col. 4, line 57 - co	ol. 6,line 55)	
A,P	US 5,555,366 A (TEIG et al.) 10 Se	ptember 1996, (abstract,	1,2
	fig. 8, fig. 12)		
		1002 (20)	1,2
Α	US 5,265,030 A (SKOLNICK et al.)	23 November 1993, (co.	1,2
	2, line 20 - col. 3, line 20)		
1	MAGARTIN "Small Pontide De	signed that can Mimic	1-6
A,P	MCCARTHY, "Small Peptide De Erythropoietin" Lancet, 8/96 vol.	348 no. 24. n.395	
	Erythropoletin Lancet, 9/30 voi.	040, no. 2 1, pro-	
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INTERNATIONAL SEARCH REPORT

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